Tricosane

Other names: n-Tricosane
Inchi: InChI=1S/C23H48/c1-3-5-7-9-11-13-15-17-19-21-23-22-20-18-16-14-12-10-8-6-4-2/h3-23
InchiKey: FIGVVZUWCLSUEI-UHFFFAOYSA-N
Formula: C23H48
SMILES: CCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 324.63
CAS: 638-67-5

Physical Properties

Property code	Value	Unit	Source
gf	142.78	kJ/mol	Joback Method
hf	-518.05	kJ/mol	Joback Method
hfus	55.33	kJ/mol	Joback Method
hvap	117.00	kJ/mol	NIST Webbook
hvap	119.70 ± 2.30	kJ/mol	NIST Webbook
hvap	118.70 ± 0.10	kJ/mol	NIST Webbook
hvap	120.50 ± 2.00	kJ/mol	NIST Webbook
log10ws	-9.45		Crippen Method
logp	9.218		Crippen Method
mcvol	334.930	ml/mol	McGowan Method
pc	920.00	kPa	KDB
pc	915.00 ± 40.00	kPa	NIST Webbook
pc	900.00 ± 200.00	kPa	NIST Webbook
rinpol	388.70		NIST Webbook
rinpol	369.44		NIST Webbook
rinpol	388.70		NIST Webbook
rinpol	388.80		NIST Webbook
rinpol	369.44		NIST Webbook
rinpol	376.29		NIST Webbook
tb	593.90 ± 2.00	K	NIST Webbook
tb	653.20	K	NIST Webbook
tc	791.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tc	790.00 ± 8.00	K	NIST Webbook
tc	789.70 ± 3.00	K	NIST Webbook

tc	790.00	K	KDB
tf	320.57 ± 0.30	K	NIST Webbook
tf	321.00 ± 2.00	K	NIST Webbook
tf	320.00 ± 2.00	K	NIST Webbook
tf	317.30 ± 3.00	K	NIST Webbook
tf	319.00 ± 3.00	K	NIST Webbook
tf	321.00 ± 6.00	K	NIST Webbook
tf	320.50 ± 0.50	K	NIST Webbook
tf	320.90 ± 2.00	K	NIST Webbook
tf	320.90 ± 1.00	K	NIST Webbook
tf	319.00 ± 2.00	K	NIST Webbook
tf	320.47 ± 0.40	K	NIST Webbook
tf	320.00 ± 2.00	K	NIST Webbook
tf	320.20 ± 0.60	K	NIST Webbook
tf	320.75 ± 0.15	K	NIST Webbook
tf	320.70 ± 0.30	K	NIST Webbook
tf	320.50 ± 0.25	K	NIST Webbook
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.30	J/mol×K	725.64	Joback Method
cpg	1046.59	J/mol×K	753.36	Joback Method
cpg	1067.91	J/mol×K	781.09	Joback Method
cpg	1088.30	J/mol×K	808.81	Joback Method
cpg	1107.77	J/mol×K	836.54	Joback Method
cpg	1126.37	J/mol×K	864.26	Joback Method
cpg	1144.12	J/mol×K	891.98	Joback Method
cpl	772.00	J/mol×K	353.00	NIST Webbook
dvisc	0.0026300	Pa×s	348.97	Joback Method
dvisc	0.0000914	Pa×s	662.86	Joback Method
dvisc	0.0000661	Pa×s	725.64	Joback Method
dvisc	0.0002187	Pa×s	537.31	Joback Method
dvisc	0.0004023	Pa×s	474.53	Joback Method
dvisc	0.0008915	Pa×s	411.75	Joback Method
dvisc	0.0001350	Pa×s	600.08	Joback Method
hfust	52.60	kJ/mol	320.20	NIST Webbook
hfust	53.97	kJ/mol	320.70	NIST Webbook
hfust	76.70	kJ/mol	319.70	NIST Webbook
hfust	21.76	kJ/mol	313.70	NIST Webbook

hfust	53.97	kJ/mol	320.70	NIST Webbook
hvapt	93.50	kJ/mol	437.00	NIST Webbook
hvapt	117.00	kJ/mol	298.15	Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C21 to C30 at T = 298.15 K by Correlation Gas Chromatography
hvapt	94.00	kJ/mol	546.50	NIST Webbook
hvapt	110.40	kJ/mol	333.50	NIST Webbook
hvapt	92.00	kJ/mol	430.00	NIST Webbook
hvapt	123.00 ± 1.00	kJ/mol	393.00	NIST Webbook
pvap	0.24	kPa	461.99	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.01	kPa	412.18	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.02	kPa	422.26	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.02	kPa	422.29	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.05	kPa	432.34	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K

pvap	0.08	kPa	442.33	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.14	kPa	452.22	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
sfust	239.90	J/mol×K	319.70	NIST Webbook
sfust	69.37	J/mol×K	313.70	NIST Webbook
sfust	168.33	J/mol×K	320.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	472.70	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.05833e+02
Coeff. B	-2.71788e+04
Coeff. C	-4.10052e+01
Coeff. D	1.44985e-05
Temperature range (K), min.	440.15
Temperature range (K), max.	653.15

Sources

Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C21 to C30 at T = 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0301747
Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique:	https://www.doi.org/10.1016/j.fluid.2014.07.017
KDB:	https://www.cheric.org/files/research/kdb/mol/mol23.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=23
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K:	https://www.doi.org/10.1021/je050182i

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume