

12-Methyltricosane

Other names:	Tricosane, 12-methyl
Inchi:	InChI=1S/C24H50/c1-4-6-8-10-12-14-16-18-20-22-24(3)23-21-19-17-15-13-11-9-7-5-2/h2
InchiKey:	RDTOGNLPXWGYBE-UHFFFAOYSA-N
Formula:	C24H50
SMILES:	CCCCCCCCCCCC(C)CCCCCCCCCCC
Mol. weight [g/mol]:	338.65
CAS:	22331-52-8

Physical Properties

Property code	Value	Unit	Source
af	0.9558		Cheméo Relay (1.0)
gf	148.76	kJ/mol	Joback Method
hf	-549.65	kJ/mol	Cheméo Relay (1.0)
hfus	54.39	kJ/mol	Joback Method
hvap	113.97	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	Cheméo Relay (1.0)
log10ws	-9.66		Cheméo Relay (1.0)
logp	9.464		Crippen Method
mcvol	349.020	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
tb	601.39	K	Cheméo Relay (1.0)
tc	770.30	K	Cheméo Relay (1.0)
tf	288.19	K	Cheméo Relay (1.0)
vc	1.376	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.86	J/mol×K	748.08	Joback Method
cpg	1210.52	J/mol×K	918.22	Joback Method
cpg	1192.43	J/mol×K	889.86	Joback Method
cpg	1173.45	J/mol×K	861.51	Joback Method
cpg	1153.54	J/mol×K	833.15	Joback Method
cpg	1132.66	J/mol×K	804.79	Joback Method

cpg	1110.78	J/mol×K	776.44	Joback Method
dvisc	0.0001924	Pa×s	546.66	Joback Method
dvisc	0.0000532	Pa×s	748.08	Joback Method
dvisc	0.0000751	Pa×s	680.94	Joback Method
dvisc	0.0001142	Pa×s	613.80	Joback Method
dvisc	0.0031119	Pa×s	345.24	Joback Method
dvisc	0.0003752	Pa×s	479.52	Joback Method
dvisc	0.0009096	Pa×s	412.38	Joback Method
hvapt	84.50	kJ/mol	444.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.00814e+01
Coeff. B	-1.01663e+04
Temperature range (K), min.	513.61
Temperature range (K), max.	688.31

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22331528&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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