1-TRICOSENE

Other names: Tricosene-1
Inchi: InChI=1S/C23H46/c1-3-5-7-9-11-13-15-17-19-21-23-22-20-18-16-14-12-10-8-6-4-2/h3H,
InchiKey: SJDSOBWGZRPKSB-UHFFFAOYSA-N
Formula: C23H46
SMILES: C=CCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 322.62
CAS: 18835-32-0

Physical Properties

Property code	Value	Unit	Source
af	0.9304		Cheméo Relay (1.0)
gf	230.62	kJ/mol	Joback Method
hf	-408.93	kJ/mol	Cheméo Relay (1.0)
hfus	54.05	kJ/mol	Joback Method
hvap	113.82	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-9.14		Cheméo Relay (1.0)
logp	8.994		Crippen Method
mcvol	330.630	ml/mol	McGowan Method
pc	873.25	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2288.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2289.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	620.92	K	Cheméo Relay (1.0)
tc	774.23	K	Cheméo Relay (1.0)
tf	305.65	K	Cheméo Relay (1.0)
vc	1.312	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.72	J/mol×K	722.32	Joback Method
cpg	1020.48	J/mol×K	750.12	Joback Method
cpg	1041.29	J/mol×K	777.91	Joback Method
cpg	1061.17	J/mol×K	805.71	Joback Method
cpg	1080.17	J/mol×K	833.50	Joback Method
cpg	1098.31	J/mol×K	861.30	Joback Method
cpg	1115.65	J/mol×K	889.09	Joback Method
dvisc	0.0025755	Pa×s	347.21	Joback Method
dvisc	0.0008927	Pa×s	409.73	Joback Method
dvisc	0.0004096	Pa×s	472.25	Joback Method
dvisc	0.0002255	Pa×s	534.76	Joback Method
dvisc	0.0001407	Pa×s	597.28	Joback Method
dvisc	0.0000960	Pa×s	659.80	Joback Method
dvisc	0.0000700	Pa×s	722.32	Joback Method
hvapt	98.50	kJ/mol	530.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41013e+01
Coeff. B	-4.46927e+03
Coeff. C	-1.73053e+02
Temperature range (K), min.	496.59
Temperature range (K), max.	681.51

Sources

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
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=C18835320&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume