Eicosane, 3-cyclohexyl-

Other names: 3-Cyclohexyleicosane
Inchi: InChI=1S/C26H52/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-25(4-2)26-23-20-18-21
InchiKey: PANSPXWYXYRKGU-UHFFFAOYSA-N
Formula: C26H52
SMILES: CCCCCCCCCCCCCCCCCC(CC)C1CCCCC1
Mol. weight [g/mol]: 364.69
CAS: 4443-57-6

Physical Properties

Property code	Value	Unit	Source
chl	-16996.70 ± 6.70	kJ/mol	NIST Webbook
gf	190.05	kJ/mol	Joback Method
hf	-530.93	kJ/mol	Joback Method
hfl	-666.20 ± 6.70	kJ/mol	NIST Webbook
hfus	51.41	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-10.12		Crippen Method
logp	9.854		Crippen Method
mcvol	366.340	ml/mol	McGowan Method
pc	815.86	kPa	Joback Method
tb	813.39	K	Joback Method
tc	999.44	K	Joback Method
tf	295.85 ± 0.50	K	NIST Webbook
tf	295.90 ± 0.50	K	NIST Webbook
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1217.92	J/mol×K	813.39	Joback Method
cpg	1242.43	J/mol×K	844.40	Joback Method
cpg	1265.60	J/mol×K	875.41	Joback Method
cpg	1287.48	J/mol×K	906.41	Joback Method
cpg	1308.14	J/mol×K	937.42	Joback Method

cpg	1327.62	J/mol×K	968.43	Joback Method
cpg	1345.98	J/mol×K	999.44	Joback Method
dvisc	0.0027649	Pa×s	375.16	Joback Method
dvisc	0.0007775	Pa×s	448.20	Joback Method
dvisc	0.0003120	Pa×s	521.24	Joback Method
dvisc	0.0001567	Pa×s	594.27	Joback Method
dvisc	0.0000915	Pa×s	667.31	Joback Method
dvisc	0.0000594	Pa×s	740.35	Joback Method
dvisc	0.0000417	Pa×s	813.39	Joback Method
hvapt	94.00	kJ/mol	511.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49969e+01
Coeff. B	-5.71965e+03
Coeff. C	-1.32873e+02
Temperature range (K), min.	521.72
Temperature range (K), max.	723.42

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4443576&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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