

Hexatriacontane, 5,13,17-trimethyl

Inchi:	InChI=1S/C39H80/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-24-27-33-38(4)35-39
InchiKey:	PAXVFNQSYSLPHZ-UHFFFAOYSA-N
Formula:	C39H80
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC(C)CCCC
Mol. weight [g/mol]:	549.05

Physical Properties

Property code	Value	Unit	Source
gf	270.18	kJ/mol	Joback Method
hf	-864.13	kJ/mol	Joback Method
hfus	86.20	kJ/mol	Joback Method
hvap	101.24	kJ/mol	Joback Method
log10ws	-15.42		Crippen Method
logp	15.028		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	410.11	kPa	Joback Method
rinsol	3697.00		NIST Webbook
tb	1090.40	K	Joback Method
tc	1421.58	K	Joback Method
tf	484.29	K	Joback Method
vc	2.201	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.46	J/molxK	1090.40	Joback Method
cpg	2144.50	J/molxK	1145.60	Joback Method
cpg	2180.17	J/molxK	1200.79	Joback Method
cpg	2212.89	J/molxK	1255.99	Joback Method
cpg	2243.14	J/molxK	1311.19	Joback Method
cpg	2271.37	J/molxK	1366.39	Joback Method
cpg	2298.04	J/molxK	1421.58	Joback Method
dvisc	0.0004814	Paxs	484.29	Joback Method
dvisc	0.0001118	Paxs	585.31	Joback Method

dvisc	0.0000399	Paxs	686.33	Joback Method
dvisc	0.0000186	Paxs	787.35	Joback Method
dvisc	0.0000103	Paxs	888.36	Joback Method
dvisc	0.0000064	Paxs	989.38	Joback Method
dvisc	0.0000044	Paxs	1090.40	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R584282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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