Hexatriacontane, 12,16,20-trimethyl

Inchi: InChI=1S/C39H80/c1-6-8-10-12-14-16-17-18-19-20-22-24-26-28-32-38(4)34-30-36-39(5)35-31-37(3)33-29-27-25-23-21-15-13-11-9-7-2/h37-39H,6-36H2,1-5H3

InchiKey: CTWSHBJMNATGHS-UHFFFAOYSA-N

Formula: C39H80

SMILES: CCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCC

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
rinpol	3677.00		NIST Webbook
rinpol	3677.00		NIST Webbook
tb	1090.40	K	Joback Method
tc	1421.58	K	Joback Method
tf	484.29	K	Joback Method
vc	2.201	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.46	J/mol×K	1090.40	Joback Method
cpg	2271.37	J/mol×K	1366.39	Joback Method
cpg	2243.14	J/mol×K	1311.19	Joback Method
cpg	2212.89	J/mol×K	1255.99	Joback Method
cpg	2180.17	J/mol×K	1200.79	Joback Method
cpg	2144.50	J/mol×K	1145.60	Joback Method
cpg	2298.04	J/mol×K	1421.58	Joback Method
dvisc	0.0000044	Pa×s	1090.40	Joback Method

dvisc	0.0000064	Pa×s	989.38	Joback Method
dvisc	0.0000103	Pa×s	888.36	Joback Method
dvisc	0.0000186	Pa×s	787.35	Joback Method
dvisc	0.0000399	Pa×s	686.33	Joback Method
dvisc	0.0001118	Pa×s	585.31	Joback Method
dvisc	0.0004814	Pa×s	484.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R584237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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