

Hexatriacontane, 13,17-dimethyl

Inchi:	InChI=1S/C38H78/c1-5-7-9-11-13-15-17-18-19-20-21-22-23-25-27-29-31-34-38(4)36-32
InchiKey:	SJRJLTVEOINAGW-UHFFFAOYSA-N
Formula:	C38H78
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	535.03

Physical Properties

Property code	Value	Unit	Source
gf	264.20	kJ/mol	Joback Method
hf	-838.21	kJ/mol	Joback Method
hfus	87.13	kJ/mol	Joback Method
hvap	99.41	kJ/mol	Joback Method
log10ws	-15.25		Crippen Method
logp	14.782		Crippen Method
mcvol	546.280	ml/mol	McGowan Method
pc	425.12	kPa	Joback Method
rinpol	3649.00		NIST Webbook
tb	1067.96	K	Joback Method
tc	1383.24	K	Joback Method
tf	488.02	K	Joback Method
vc	2.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2035.13	J/molxK	1067.96	Joback Method
cpg	2196.76	J/molxK	1330.69	Joback Method
cpg	2169.20	J/molxK	1278.14	Joback Method
cpg	2139.64	J/molxK	1225.60	Joback Method
cpg	2107.70	J/molxK	1173.05	Joback Method
cpg	2072.99	J/molxK	1120.51	Joback Method
cpg	2222.69	J/molxK	1383.24	Joback Method
dvisc	0.0000057	Paxs	1067.96	Joback Method
dvisc	0.0000082	Paxs	971.30	Joback Method

dvisc	0.0000129	Paxs	874.65	Joback Method
dvisc	0.0000227	Paxs	777.99	Joback Method
dvisc	0.0000467	Paxs	681.33	Joback Method
dvisc	0.0001222	Paxs	584.68	Joback Method
dvisc	0.0004682	Paxs	488.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R584262&Units=SI

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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