Hexatriacontane, 12,16-dimethyl

Other names: 12,16-Dimethylhexatriacontane
Inchi: InChI=1S/C38H78/c1-5-7-9-11-13-15-16-17-18-19-20-21-22-23-25-27-29-31-34-38(4)36-
InchiKey: INQHCWWNHXTNPH-UHFFFAOYSA-N
Formula: C38H78
SMILES: CCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCC
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	3666.00		NIST Webbook
rinpol	3652.00		NIST Webbook
rinpol	3652.00		NIST Webbook
rinpol	3666.00		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/mol×K	1067.96	Joback Method
cpg	2196.76	J/mol×K	1330.69	Joback Method
cpg	2169.20	J/mol×K	1278.14	Joback Method
cpg	2139.64	J/mol×K	1225.60	Joback Method
cpg	2107.70	J/mol×K	1173.05	Joback Method

cpg	2072.99	J/mol×K	1120.51	Joback Method
cpg	2222.69	J/mol×K	1383.24	Joback Method
dvisc	0.0000057	Pa×s	1067.96	Joback Method
dvisc	0.0000082	Pa×s	971.30	Joback Method
dvisc	0.0000129	Pa×s	874.65	Joback Method
dvisc	0.0000227	Pa×s	777.99	Joback Method
dvisc	0.0000467	Pa×s	681.33	Joback Method
dvisc	0.0001222	Pa×s	584.68	Joback Method
dvisc	0.0004682	Pa×s	488.02	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R337432&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