13,17,21-Trimethyltritriacontane

Inchi: InChI=1S/C36H74/c1-6-8-10-12-14-16-18-20-22-24-28-34(3)30-26-32-36(5)33-27-31-35(
InchiKey: VPNSAYIYZOPVGL-UHFFFAOYSA-N
Formula: C36H74
SMILES: CCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]: 506.97
CAS: 58668-38-5

Physical Properties

Property code	Value	Unit	Source
gf	244.92	kJ/mol	Joback Method
hf	-802.21	kJ/mol	Joback Method
hfus	78.43	kJ/mol	Joback Method
hvap	94.57	kJ/mol	Joback Method
log10ws	-14.17		Crippen Method
logp	13.857		Crippen Method
mcvol	518.100	ml/mol	McGowan Method
pc	462.48	kPa	Joback Method
rinpol	3375.00		NIST Webbook
rinpol	3379.00		NIST Webbook
rinpol	3377.00		NIST Webbook
tb	1021.76	K	Joback Method
tc	1294.81	K	Joback Method
tf	450.48	K	Joback Method
vc	2.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1895.31	J/mol×K	1021.76	Joback Method
cpg	1929.03	J/mol×K	1067.27	Joback Method
cpg	1960.20	J/mol×K	1112.78	Joback Method
cpg	1989.08	J/mol×K	1158.29	Joback Method
cpg	2015.88	J/mol×K	1203.80	Joback Method
cpg	2040.85	J/mol×K	1249.30	Joback Method

cpg	2064.22	J/mol×K	1294.81	Joback Method
dvisc	0.0008138	Pa×s	450.48	Joback Method
dvisc	0.0001858	Pa×s	545.69	Joback Method
dvisc	0.0000658	Pa×s	640.91	Joback Method
dvisc	0.0000305	Pa×s	736.12	Joback Method
dvisc	0.0000168	Pa×s	831.33	Joback Method
dvisc	0.0000105	Pa×s	926.55	Joback Method
dvisc	0.0000072	Pa×s	1021.76	Joback Method

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=C58668385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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