5,17-Dimethyloctatriacontane

Other names: Octatriacontane, 5,17-dimethyl
Inchi: InChI=1S/C40H82/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-23-26-30-33-37-40(4)
InchiKey: WGGKMOFKTFLGML-UHFFFAOYSA-N
Formula: C40H82
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]: 563.08

Physical Properties

Property code	Value	Unit	Source
gf	281.04	kJ/mol	Joback Method
hf	-879.49	kJ/mol	Joback Method
hfus	92.31	kJ/mol	Joback Method
hvap	103.86	kJ/mol	Joback Method
log10ws	-16.08		Crippen Method
logp	15.562		Crippen Method
mcvol	574.460	ml/mol	McGowan Method
pc	393.36	kPa	Joback Method
rinpol	3878.00		NIST Webbook
rinpol	3878.00		NIST Webbook
rinpol	3880.00		NIST Webbook
tb	1113.72	K	Joback Method
tc	1475.80	K	Joback Method
tf	510.56	K	Joback Method
vc	2.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2176.00	J/mol×K	1113.72	Joback Method
cpg	2218.14	J/mol×K	1174.07	Joback Method
cpg	2256.46	J/mol×K	1234.41	Joback Method
cpg	2291.57	J/mol×K	1294.76	Joback Method
cpg	2324.07	J/mol×K	1355.11	Joback Method
cpg	2354.59	J/mol×K	1415.45	Joback Method

cpg	2383.72	J/mol×K	1475.80	Joback Method
dvisc	0.0003343	Pa×s	510.56	Joback Method
dvisc	0.0000877	Pa×s	611.09	Joback Method
dvisc	0.0000336	Pa×s	711.61	Joback Method
dvisc	0.0000163	Pa×s	812.14	Joback Method
dvisc	0.0000093	Pa×s	912.67	Joback Method
dvisc	0.0000059	Pa×s	1013.19	Joback Method
dvisc	0.0000041	Pa×s	1113.72	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R505605&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

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