9,13,17,21-Tetramethylpentatriacontane

Inchi: InChI=1S/C39H80/c1-7-9-11-13-15-16-17-18-19-20-22-24-29-37(4)31-26-33-39(6)35-27-
InchiKey: NAODCCFDOIDWOA-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCC
Mol. weight [g/mol]: 549.05

Physical Properties

Property code	Value	Unit	Source
gf	267.74	kJ/mol	Joback Method
hf	-869.41	kJ/mol	Joback Method
hfus	82.67	kJ/mol	Joback Method
hvap	100.86	kJ/mol	Joback Method
log10ws	-15.18		Crippen Method
logp	14.883		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	411.44	kPa	Joback Method
rinpol	3617.00		NIST Webbook
rinpol	3617.00		NIST Webbook
rinpol	3617.00		NIST Webbook
tb	1089.96	K	Joback Method
tc	1415.10	K	Joback Method
tf	469.29	K	Joback Method
vc	2.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.45	J/mol×K	1089.96	Joback Method
cpg	2267.84	J/mol×K	1360.91	Joback Method
cpg	2240.25	J/mol×K	1306.72	Joback Method
cpg	2210.65	J/mol×K	1252.53	Joback Method
cpg	2178.60	J/mol×K	1198.34	Joback Method
cpg	2143.68	J/mol×K	1144.15	Joback Method
cpg	2293.84	J/mol×K	1415.10	Joback Method

dvisc	0.0000040	Pa×s	1089.96	Joback Method
dvisc	0.0000059	Pa×s	986.51	Joback Method
dvisc	0.0000096	Pa×s	883.07	Joback Method
dvisc	0.0000179	Pa×s	779.62	Joback Method
dvisc	0.0000404	Pa×s	676.18	Joback Method
dvisc	0.0001218	Pa×s	572.74	Joback Method
dvisc	0.0005981	Pa×s	469.29	Joback Method

Sources

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=R505907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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