Octatriacontane, 17-methyl

Inchi: InChI=1S/C39H80/c1-4-6-8-10-12-14-16-18-20-21-22-23-24-26-28-30-32-34-36-38-39(3)
InchiKey: IIIFHZNRMYPHAO-UHFFFAOYSA-N
Formula: C39H80
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 549.05

Physical Properties

Property code	Value	Unit	Source
gf	275.06	kJ/mol	Joback Method
hf	-853.57	kJ/mol	Joback Method
hfus	93.24	kJ/mol	Joback Method
hvap	102.02	kJ/mol	Joback Method
log10ws	-15.91		Crippen Method
logp	15.316		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	407.46	kPa	Joback Method
rinpol	3822.00		NIST Webbook
tb	1091.28	K	Joback Method
tc	1435.32	K	Joback Method
tf	514.29	K	Joback Method
vc	2.213	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.47	J/mol×K	1091.28	Joback Method
cpg	2146.26	J/mol×K	1148.62	Joback Method
cpg	2183.49	J/mol×K	1205.96	Joback Method
cpg	2217.67	J/mol×K	1263.30	Joback Method
cpg	2249.30	J/mol×K	1320.64	Joback Method
cpg	2278.91	J/mol×K	1377.98	Joback Method
cpg	2306.99	J/mol×K	1435.32	Joback Method
dvisc	0.0003317	Pa×s	514.29	Joback Method
dvisc	0.0000968	Pa×s	610.45	Joback Method

dvisc	0.0000395	Pa×s	706.62	Joback Method
dvisc	0.0000200	Pa×s	802.78	Joback Method
dvisc	0.0000117	Pa×s	898.95	Joback Method
dvisc	0.0000076	Pa×s	995.12	Joback Method
dvisc	0.0000053	Pa×s	1091.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R584386&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

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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