

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:	CCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCC
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/molxK	1091.28	Joback Method
cpg	2146.26	J/molxK	1148.62	Joback Method
cpg	2183.49	J/molxK	1205.96	Joback Method
cpg	2217.67	J/molxK	1263.30	Joback Method
cpg	2249.30	J/molxK	1320.64	Joback Method
cpg	2278.91	J/molxK	1377.98	Joback Method
cpg	2306.99	J/molxK	1435.32	Joback Method
dvisc	0.0003317	Paxs	514.29	Joback Method
dvisc	0.0000968	Paxs	610.45	Joback Method

dvisc	0.0000395	Paxs	706.62	Joback Method
dvisc	0.0000200	Paxs	802.78	Joback Method
dvisc	0.0000117	Paxs	898.95	Joback Method
dvisc	0.0000076	Paxs	995.12	Joback Method
dvisc	0.0000053	Paxs	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/ci9903071
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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