

Octatriacontane, 12,16-dimethyl

Inchi: InChI=1S/C40H82/c1-5-7-9-11-13-15-16-17-18-19-20-21-22-23-24-25-27-29-31-33-36-40
InchiKey: LVHAIFJVJXFDSL-UHFFFAOYSA-N
Formula: C40H82
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCC
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
mvol	574.460	ml/mol	McGowan Method
pc	393.36	kPa	Joback Method
rinpol	3852.00		NIST Webbook
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tb	1113.72	K	Joback Method
tc	1475.80	K	Joback Method
tf	510.56	K	Joback Method
vc	2.264	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2176.00	J/molxK	1113.72	Joback Method
cpg	2354.59	J/molxK	1415.45	Joback Method
cpg	2324.07	J/molxK	1355.11	Joback Method
cpg	2291.57	J/molxK	1294.76	Joback Method
cpg	2256.46	J/molxK	1234.41	Joback Method
cpg	2218.14	J/molxK	1174.07	Joback Method
cpg	2383.72	J/molxK	1475.80	Joback Method
dvisc	0.0000041	Paxs	1113.72	Joback Method

dvisc	0.0000059	Paxs	1013.19	Joback Method
dvisc	0.0000093	Paxs	912.67	Joback Method
dvisc	0.0000163	Paxs	812.14	Joback Method
dvisc	0.0000336	Paxs	711.61	Joback Method
dvisc	0.0000877	Paxs	611.09	Joback Method
dvisc	0.0003343	Paxs	510.56	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=R584366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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