

3,9-Dimethylhentriacontane

Inchi: InChI=1S/C33H68/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-30-33
InchiKey: LLZYIGVNUBLMOP-UHFFFAOYSA-N
Formula: C33H68
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCCC(C)CC
Mol. weight [g/mol]: 464.89

Physical Properties

Property code	Value	Unit	Source
gf	222.10	kJ/mol	Joback Method
hf	-735.01	kJ/mol	Joback Method
hfus	74.18	kJ/mol	Joback Method
hvap	88.28	kJ/mol	Joback Method
log10ws	-13.15		Crippen Method
logp	12.831		Crippen Method
mcvol	475.830	ml/mol	McGowan Method
pc	523.65	kPa	Joback Method
rinpol	3208.00		NIST Webbook
rinpol	3203.00		NIST Webbook
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
rinpol	3209.00		NIST Webbook
rinpol	3210.00		NIST Webbook
rinpol	3207.00		NIST Webbook
rinpol	3209.00		NIST Webbook
tb	953.56	K	Joback Method
tc	1187.32	K	Joback Method
tf	431.67	K	Joback Method
vc	1.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1687.29	J/mol×K	953.56	Joback Method
cpg	1819.42	J/mol×K	1148.36	Joback Method

cpg	1796.37	J/mol×K	1109.40	Joback Method
cpg	1771.77	J/mol×K	1070.44	Joback Method
cpg	1745.48	J/mol×K	1031.48	Joback Method
cpg	1717.36	J/mol×K	992.52	Joback Method
cpg	1841.06	J/mol×K	1187.32	Joback Method
dvisc	0.0000127	Pa×s	953.56	Joback Method
dvisc	0.0000184	Pa×s	866.58	Joback Method
dvisc	0.0000288	Pa×s	779.60	Joback Method
dvisc	0.0000506	Pa×s	692.62	Joback Method
dvisc	0.0001044	Pa×s	605.63	Joback Method
dvisc	0.0002747	Pa×s	518.65	Joback Method
dvisc	0.0010674	Pa×s	431.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R262016&Units=SI

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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