

3,13-Dimethylhentriacontane

Inchi: InChI=1S/C33H68/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-20-24-27-30-33(4)31-28-25-2
InchiKey: GTJQKNJBNNGPRN-UHFFFAOYSA-N
Formula: C33H68
SMILES: CCCCCCCCCCCCCCCCCC(C)CCCCCCCCC(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	3204.00		NIST Webbook
rinpol	3204.00		NIST Webbook
rinpol	3204.00		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/molxK	953.56	Joback Method
cpg	1819.42	J/molxK	1148.36	Joback Method
cpg	1796.37	J/molxK	1109.40	Joback Method
cpg	1771.77	J/molxK	1070.44	Joback Method
cpg	1745.48	J/molxK	1031.48	Joback Method
cpg	1717.36	J/molxK	992.52	Joback Method
cpg	1841.06	J/molxK	1187.32	Joback Method

dvisc	0.0000127	Paxs	953.56	Joback Method
dvisc	0.0000184	Paxs	866.58	Joback Method
dvisc	0.0000288	Paxs	779.60	Joback Method
dvisc	0.0000506	Paxs	692.62	Joback Method
dvisc	0.0001044	Paxs	605.63	Joback Method
dvisc	0.0002747	Paxs	518.65	Joback Method
dvisc	0.0010674	Paxs	431.67	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=R505358&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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