(S)11,21-dimethyl-hentriacontane

Inchi: InChI=1S/C33H68/c1-5-7-9-11-13-16-20-24-28-32(3)30-26-22-18-15-19-23-27-31-33(4)2
InchiKey: CJFUDEXKMZHMRN-CZNDPXEESA-N
Formula: C33H68
SMILES: CCCCCCCCCCC(C)CCCCCCCCCC(C)CCCCCCCCC
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	3163.00		NIST Webbook
rinpol	3163.00		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	1717.36	J/mol×K	992.52	Joback Method
cpg	1745.48	J/mol×K	1031.48	Joback Method
cpg	1771.77	J/mol×K	1070.44	Joback Method
cpg	1796.37	J/mol×K	1109.40	Joback Method
cpg	1819.42	J/mol×K	1148.36	Joback Method
cpg	1841.06	J/mol×K	1187.32	Joback Method
dvisc	0.0010674	Pa×s	431.67	Joback Method

dvisc	0.0002747	Pa×s	518.65	Joback Method
dvisc	0.0001044	Pa×s	605.63	Joback Method
dvisc	0.0000506	Pa×s	692.62	Joback Method
dvisc	0.0000288	Pa×s	779.60	Joback Method
dvisc	0.0000184	Pa×s	866.58	Joback Method
dvisc	0.0000127	Pa×s	953.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R300673&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