

(4E)-3,6,9,10,13,14-hexamethyl-3-(3,4,7,8-tetramet

Inchi: InChI=1S/C33H64/c1-13-26(5)15-17-30(9)32(11)22-24-33(12,14-2)23-21-27(6)16-18-29(4)
InchiKey: NBOHZPQWJWZHLT-XTQSDGFTSA-N
Formula: C33H64
SMILES: C=CC(C)(C=CC(C)CCC(C)C(C)CCC(C)C(C)C)CCC(C)C(C)CCC(C)CC
Mol. weight [g/mol]: 460.86

Physical Properties

Property code	Value	Unit	Source
gf	378.36	kJ/mol	Joback Method
hf	-532.79	kJ/mol	Joback Method
hfus	44.55	kJ/mol	Joback Method
hvap	83.94	kJ/mol	Joback Method
log10ws	-11.17		Crippen Method
logp	11.374		Crippen Method
mcvol	467.230	ml/mol	McGowan Method
pc	564.47	kPa	Joback Method
rinpol	2761.00		NIST Webbook
rinpol	2761.00		NIST Webbook
tb	948.53	K	Joback Method
tc	1162.60	K	Joback Method
tf	337.25	K	Joback Method
vc	1.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1630.81	J/molxK	948.53	Joback Method
cpg	1657.26	J/molxK	984.21	Joback Method
cpg	1682.29	J/molxK	1019.89	Joback Method
cpg	1706.05	J/molxK	1055.56	Joback Method
cpg	1728.66	J/molxK	1091.24	Joback Method
cpg	1750.28	J/molxK	1126.92	Joback Method
cpg	1771.04	J/molxK	1162.60	Joback Method
dvisc	0.0086511	Paxs	337.25	Joback Method

dvisc	0.0006030	Paxs	439.13	Joback Method
dvisc	0.0001146	Paxs	541.01	Joback Method
dvisc	0.0000369	Paxs	642.89	Joback Method
dvisc	0.0000162	Paxs	744.77	Joback Method
dvisc	0.0000087	Paxs	846.65	Joback Method
dvisc	0.0000053	Paxs	948.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586466&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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