

5-[(4E)-3,6-dimethyl-6-(3,4,7,8-tetramethylnonyl)-4

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C34H62/c1-14-34(13,22-20-28(7)27(6)17-16-26(5)24(2)3)21-19-25(4)15-18-32

LLSLXMBBDWBAAH-XUTLUUPISA-N

C34H62

C=CC(C)(C=CC(C)CCC1C(C)C(C)=CC(C)C1(C)C)CCC(C)C(C)CCC(C)C(C)C

470.86

Physical Properties

Property code	Value	Unit	Source
gf	410.26	kJ/mol	Joback Method
hf	-482.74	kJ/mol	Joback Method
hfus	47.29	kJ/mol	Joback Method
hvap	86.63	kJ/mol	Joback Method
log10ws	-11.09		Crippen Method
logp	11.150		Crippen Method
mcvol	466.160	ml/mol	McGowan Method
pc	578.68	kPa	Joback Method
rinpol	2796.00		NIST Webbook
tb	982.65	K	Joback Method
tc	1203.05	K	Joback Method
tf	425.36	K	Joback Method
vc	1.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1682.17	J/mol×K	982.65	Joback Method
cpg	1712.35	J/mol×K	1019.38	Joback Method
cpg	1741.85	J/mol×K	1056.12	Joback Method
cpg	1770.87	J/mol×K	1092.85	Joback Method
cpg	1799.64	J/mol×K	1129.58	Joback Method
cpg	1828.37	J/mol×K	1166.31	Joback Method
cpg	1857.28	J/mol×K	1203.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586471&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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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