5-{(4E)-3,6-dimethyl-6-[3-(3,3,4-trimethyl-1-cycloh
Isomer # 1

Inchi: InChI=1S/C34H58/c1-13-34(12,21-19-25(3)30-16-15-27(5)32(8,9)23-30)20-18-24(2)14-1
InchiKey: WBWJFIXPBMQEDE-CZIZESTLSA-N
Formula: C34H58
SMILES: C=CC(C)(C=CC(C)CCC1C(C)C(C)=CC(C)C1(C)C)CCC(C)C1=CC(C)(C)C(C)CC1
Mol. weight [g/mol]: 466.82

Physical Properties

Property code	Value	Unit	Source
gf	449.16	kJ/mol	Joback Method
hf	-371.37	kJ/mol	Joback Method
hfus	45.30	kJ/mol	Joback Method
hvap	87.72	kJ/mol	Joback Method
log10ws	-11.08		Crippen Method
logp	10.825		Crippen Method
mcvol	451.000	ml/mol	McGowan Method
pc	643.20	kPa	Joback Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	1003.23	K	Joback Method
tc	1230.66	K	Joback Method
tf	510.68	K	Joback Method
vc	1.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1662.60	J/mol×K	1003.23	Joback Method
cpg	1697.54	J/mol×K	1041.13	Joback Method
cpg	1732.87	J/mol×K	1079.04	Joback Method
cpg	1768.92	J/mol×K	1116.94	Joback Method
cpg	1806.00	J/mol×K	1154.85	Joback Method
cpg	1844.44	J/mol×K	1192.75	Joback Method
cpg	1884.56	J/mol×K	1230.66	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=R586486&Units=SI

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