

2-{(4E)-3,6-dimethyl-6-[3-(3,3,4-trimethylcyclohexylidene)-3,6-dimethyl-5-octen-1-ylidene]-3,6-dimethyl-5-octen-1-ylidene}-3,6-dimethyl-5-octen-1-ylidene

InChI: InChI=1S/C33H56/c1-12-33(11,22-20-25(3)29-17-16-27(5)31(7,8)23-29)21-19-24(2)13-14
InChIKey: VIBZFVIDYOALBH-NMKLIDAOSA-N

Formula: C33H56
SMILES: C=CC(C)(C=CC(C)CCC1C(=C)CCC(C)C1(C)C)CCC(C)=C1CCC(C)C(C)(C)C1
Mol. weight [g/mol]: 452.80

Physical Properties

Property code	Value	Unit	Source
gf	500.22	kJ/mol	Joback Method
hf	-267.25	kJ/mol	Joback Method
hfus	41.35	kJ/mol	Joback Method
hvap	85.31	kJ/mol	Joback Method
log10ws	-11.15		Crippen Method
logp	10.723		Crippen Method
mcvol	436.910	ml/mol	McGowan Method
pc	688.53	kPa	Joback Method
rinpol	2769.00		NIST Webbook
rinpol	2769.00		NIST Webbook
tb	982.86	K	Joback Method
tc	1208.68	K	Joback Method
tf	502.17	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1587.87	J/mol×K	982.86	Joback Method
cpg	1621.95	J/mol×K	1020.50	Joback Method
cpg	1656.41	J/mol×K	1058.13	Joback Method
cpg	1691.58	J/mol×K	1095.77	Joback Method
cpg	1727.79	J/mol×K	1133.40	Joback Method
cpg	1765.37	J/mol×K	1171.04	Joback Method
cpg	1804.64	J/mol×K	1208.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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