1,1,6-trimethyl-3-methylene-2-[(4E)-3,6,13,14-tetra
Isomer # 3

Inchi: InChI=1S/C32H54/c1-12-32(11,22-13-14-25(4)15-17-27(6)24(2)3)23-21-26(5)16-20-30-2
InchiKey: DPNSRERJUWNCKU-UHFFFAOYSA-N
Formula: C32H54
SMILES: C=CC(C)(C=CC(C)CCC1C(=C)CCC(C)C1(C)C)CCCC(=C)CCC(C)C(=C)C
Mol. weight [g/mol]: 438.77

Physical Properties

Property code	Value	Unit	Source
gf	599.78	kJ/mol	Joback Method
hf	-136.07	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	81.68	kJ/mol	Joback Method
log10ws	-10.93		Crippen Method
logp	10.499		Crippen Method
mcvol	429.380	ml/mol	McGowan Method
pc	669.77	kPa	Joback Method
rinpol	2722.00		NIST Webbook
tb	931.02	K	Joback Method
tc	1142.27	K	Joback Method
tf	421.02	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1476.69	J/mol×K	931.02	Joback Method
cpg	1504.16	J/mol×K	966.23	Joback Method
cpg	1531.02	J/mol×K	1001.44	Joback Method
cpg	1557.49	J/mol×K	1036.65	Joback Method
cpg	1583.75	J/mol×K	1071.86	Joback Method
cpg	1610.01	J/mol×K	1107.06	Joback Method
cpg	1636.47	J/mol×K	1142.27	Joback Method

Sources

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=R586342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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