2,2,6-Trimethyl-6-(4-methylcyclohex-3-en-1-yl)dih

Inchi: InChI=1S/C15H24O2/c1-11-5-7-12(8-6-11)15(4)10-13(16)9-14(2,3)17-15/h5,12H,6-10H2
InchiKey: FBZSMLWLLPEEKP-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC1=CCC(C2(C)CC(=O)CC(C)(C)O2)CC1
Mol. weight [g/mol]: 236.35
CAS: 41943-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-82.75	kJ/mol	Joback Method
hf	-457.54	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	56.94	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.650		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1707.60		NIST Webbook
rinpol	1707.60		NIST Webbook
tb	676.42	K	Joback Method
tc	926.73	K	Joback Method
tf	425.20	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.76	J/mol×K	676.42	Joback Method
cpg	623.47	J/mol×K	718.14	Joback Method
cpg	646.11	J/mol×K	759.86	Joback Method
cpg	667.94	J/mol×K	801.58	Joback Method
cpg	689.24	J/mol×K	843.29	Joback Method
cpg	710.26	J/mol×K	885.01	Joback Method
cpg	731.27	J/mol×K	926.73	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=C41943811&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