Hexamethylcyclohexane-1,3,5-trione

Other names: 2,2,4,4,6,6-Hexamethyl-1,3,5-cyclohexanetrione
2,2,4,4,6,6-Hexamethylcyclohexane-1,3,5-trione
1,3,5-Cyclohexanetrione, 2,2,4,4,6,6-hexamethyl-
Inchi: InChI=1S/C12H18O3/c1-10(2)7(13)11(3,4)9(15)12(5,6)8(10)14/h1-6H3
InchiKey: DXLKLICKNIROHG-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: CC1(C)C(=O)C(C)(C)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]: 210.27
CAS: 778-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-325.05	kJ/mol	Joback Method
hf	-644.75	kJ/mol	Joback Method
hfus	0.45	kJ/mol	Joback Method
hvap	51.41	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.786		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
tb	688.35	K	Joback Method
tc	947.17	K	Joback Method
tf	500.26	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.31	J/mol×K	688.35	Joback Method
cpg	522.65	J/mol×K	731.49	Joback Method
cpg	542.76	J/mol×K	774.62	Joback Method
cpg	562.94	J/mol×K	817.76	Joback Method
cpg	583.52	J/mol×K	860.89	Joback Method
cpg	604.80	J/mol×K	904.03	Joback Method

cpg	627.08	J/mol×K	947.17	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=C778187&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume