6-Isobutyryl-2,2,4,4-tetramethylcyclohexane-1,3,5-

Other names: 1,3,5-Cyclohexanetrione, 2,2,4,4-tetramethyl-6-(2-methyl-1-oxopropyl)-
Flaveson
Flavesone
Inchi: InChI=1S/C14H20O4/c1-7(2)9(15)8-10(16)13(3,4)12(18)14(5,6)11(8)17/h7-8H,1-6H3
InchiKey: ZEOCEPNBYPGWGS-UHFFFAOYSA-N
Formula: C14H20O4
SMILES: CC(C)C(=O)C1C(=O)C(C)(C)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]: 252.31
CAS: 22595-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-434.08	kJ/mol	Joback Method
hf	-819.13	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	63.37	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.601		Crippen Method
mcvol	203.540	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
tb	787.30	K	Joback Method
tc	1035.51	K	Joback Method
tf	533.83	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.72	J/mol×K	787.30	Joback Method
cpg	659.40	J/mol×K	828.67	Joback Method
cpg	679.59	J/mol×K	870.04	Joback Method
cpg	699.46	J/mol×K	911.40	Joback Method

cpg	719.15	J/mol×K	952.77	Joback Method
cpg	738.81	J/mol×K	994.14	Joback Method
cpg	758.59	J/mol×K	1035.51	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=C22595455&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