6-acetyl-2,2,4,4-tetramethylcyclohexane-1,3,5-trio

Inchi: InChI=1S/C12H16O4/c1-6(13)7-8(14)11(2,3)10(16)12(4,5)9(7)15/h7H,1-5H3
InchiKey: AOFIHSHOAKIKPN-UHFFFAOYSA-N
Formula: C12H16O4
SMILES: CC(=O)C1C(=O)C(C)(C)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]: 224.25
CAS: 80597-59-7

Physical Properties

Property code	Value	Unit	Source
gf	-448.48	kJ/mol	Joback Method
hf	-772.57	kJ/mol	Joback Method
hfus	8.35	kJ/mol	Joback Method
hvap	59.30	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.965		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1369.30		NIST Webbook
rinpol	1369.30		NIST Webbook
tb	741.98	K	Joback Method
tc	996.11	K	Joback Method
tf	526.29	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.61	J/mol×K	741.98	Joback Method
cpg	544.71	J/mol×K	784.34	Joback Method
cpg	563.34	J/mol×K	826.69	Joback Method
cpg	581.65	J/mol×K	869.05	Joback Method
cpg	599.79	J/mol×K	911.40	Joback Method
cpg	617.92	J/mol×K	953.76	Joback Method
cpg	636.19	J/mol×K	996.11	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=C80597597&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