8-Acetoxycarvotanacetone

Inchi: InChI=1S/C12H18O3/c1-8-5-6-10(7-11(8)14)12(3,4)15-9(2)13/h5,10H,6-7H2,1-4H3
InchiKey: FTCAQUBXEGKQTD-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: CC(=O)OC(C)(C)C1CC=C(C)C(=O)C1
Mol. weight [g/mol]: 210.27
CAS: 87578-93-6

Physical Properties

Property code	Value	Unit	Source
gf	-258.73	kJ/mol	Joback Method
hf	-581.63	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.253		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1571.70		NIST Webbook
tb	638.53	K	Joback Method
tc	865.73	K	Joback Method
tf	388.46	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.92	J/mol×K	638.53	Joback Method
cpg	489.86	J/mol×K	676.40	Joback Method
cpg	506.66	J/mol×K	714.26	Joback Method
cpg	522.33	J/mol×K	752.13	Joback Method
cpg	536.87	J/mol×K	790.00	Joback Method
cpg	550.29	J/mol×K	827.86	Joback Method
cpg	562.59	J/mol×K	865.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87578936&Units=SI
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

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