Carvotanacetone, 8-acetoxy

Inchi: InChI=1S/C12H18O3/c1-8-4-5-11(6-12(8)14)9(2)7-15-10(3)13/h4,9,11H,5-7H2,1-3H3/t9?
InchiKey: PCFLUBMQGSCZOX-UMJHXOGRSA-N
Formula: C12H18O3
SMILES: CC(=O)OCC(C)C1CC=C(C)C(=O)C1
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-264.01	kJ/mol	Joback Method
hf	-578.16	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	56.70	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.111		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	641.32	K	Joback Method
tc	860.23	K	Joback Method
tf	371.04	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.41	J/mol×K	641.32	Joback Method
cpg	486.93	J/mol×K	677.81	Joback Method
cpg	503.44	J/mol×K	714.29	Joback Method
cpg	518.94	J/mol×K	750.78	Joback Method
cpg	533.41	J/mol×K	787.26	Joback Method
cpg	546.83	J/mol×K	823.75	Joback Method
cpg	559.18	J/mol×K	860.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R417815&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