Acetoxyacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C11H9NO4/c1-8(13)15-7-11(14)16-10-4-2-9(6-12)3-5-10/h2-5H,7H2,1H3
InchiKey: XSRCKJYJASEDMN-UHFFFAOYSA-N
Formula: C11H9NO4
SMILES: CC(=O)OCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 219.19

Physical Properties

Property code	Value	Unit	Source
gf	-190.14	kJ/mol	Joback Method
hf	-370.03	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	71.81	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.027		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1662.00		NIST Webbook
tb	737.40	K	Joback Method
tc	964.66	K	Joback Method
tf	461.98	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.23	J/mol×K	737.40	Joback Method
cpg	414.22	J/mol×K	775.28	Joback Method
cpg	423.40	J/mol×K	813.15	Joback Method
cpg	431.77	J/mol×K	851.03	Joback Method
cpg	439.34	J/mol×K	888.91	Joback Method
cpg	446.08	J/mol×K	926.79	Joback Method
cpg	452.00	J/mol×K	964.66	Joback Method

Sources

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=U307543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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