2,2-Dimethylpropanoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C12H13NO2/c1-12(2,3)11(14)15-10-6-4-9(8-13)5-7-10/h4-7H,1-3H3
InchiKey: KVCYRHCBMVONNS-UHFFFAOYSA-N
Formula: C12H13NO2
SMILES: CC(C)(C)C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 203.24

Physical Properties

Property code	Value	Unit	Source
gf	55.04	kJ/mol	Joback Method
hf	-154.62	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	63.58	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.510		Crippen Method
mcvol	165.000	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
tb	680.76	K	Joback Method
tc	913.60	K	Joback Method
tf	403.51	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.63	J/mol×K	680.76	Joback Method
cpg	436.28	J/mol×K	719.57	Joback Method
cpg	447.97	J/mol×K	758.37	Joback Method
cpg	458.76	J/mol×K	797.18	Joback Method
cpg	468.69	J/mol×K	835.98	Joback Method
cpg	477.82	J/mol×K	874.79	Joback Method
cpg	486.19	J/mol×K	913.60	Joback Method

Sources

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=U308043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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