Carbonic acid, isobutyl 4-cyanophenyl ester

Inchi: InChI=1S/C12H13NO3/c1-9(2)8-15-12(14)16-11-5-3-10(7-13)4-6-11/h3-6,9H,8H2,1-2H3
InchiKey: XBVVGRKZEILKCZ-UHFFFAOYSA-N
Formula: C12H13NO3
SMILES: CC(C)COC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 219.24

Physical Properties

Property code	Value	Unit	Source
gf	-55.24	kJ/mol	Joback Method
hf	-283.37	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.730		Crippen Method
mcvol	170.870	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	1703.00		NIST Webbook
tb	705.97	K	Joback Method
tc	927.78	K	Joback Method
tf	408.32	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.57	J/mol×K	705.97	Joback Method
cpg	457.84	J/mol×K	742.94	Joback Method
cpg	469.27	J/mol×K	779.91	Joback Method
cpg	479.85	J/mol×K	816.88	Joback Method
cpg	489.59	J/mol×K	853.85	Joback Method
cpg	498.49	J/mol×K	890.81	Joback Method
cpg	506.55	J/mol×K	927.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357836&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

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