Carbonic acid, butyl 4-cyanophenyl ester

Inchi: InChI=1S/C12H13NO3/c1-2-3-8-15-12(14)16-11-6-4-10(9-13)5-7-11/h4-7H,2-3,8H2,1H3
InchiKey: MPQJLBILJZIJSZ-UHFFFAOYSA-N
Formula: C12H13NO3
SMILES: CCCCOC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 219.24

Physical Properties

Property code	Value	Unit	Source
gf	-52.80	kJ/mol	Joback Method
hf	-278.09	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	67.29	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.874		Crippen Method
mcvol	170.870	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1753.00		NIST Webbook
tb	706.41	K	Joback Method
tc	924.23	K	Joback Method
tf	423.32	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.99	J/mol×K	706.41	Joback Method
cpg	457.02	J/mol×K	742.71	Joback Method
cpg	468.25	J/mol×K	779.02	Joback Method
cpg	478.67	J/mol×K	815.32	Joback Method
cpg	488.30	J/mol×K	851.63	Joback Method
cpg	497.12	J/mol×K	887.93	Joback Method
cpg	505.15	J/mol×K	924.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357850&Units=SI

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

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