Carbonic acid, ethyl 4-cyanophenyl ester

Inchi: InChI=1S/C10H9NO3/c1-2-13-10(12)14-9-5-3-8(7-11)4-6-9/h3-6H,2H2,1H3
InchiKey: QBQRNAOYCNQVFL-UHFFFAOYSA-N
Formula: C10H9NO3
SMILES: CCOC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 191.18

Physical Properties

Property code	Value	Unit	Source
gf	-69.64	kJ/mol	Joback Method
hf	-236.81	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Joback Method
hvap	62.84	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.094		Crippen Method
mcvol	142.690	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1541.00		NIST Webbook
tb	660.65	K	Joback Method
tc	886.10	K	Joback Method
tf	400.78	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.59	J/mol×K	660.65	Joback Method
cpg	356.26	J/mol×K	698.22	Joback Method
cpg	366.23	J/mol×K	735.80	Joback Method
cpg	375.50	J/mol×K	773.37	Joback Method
cpg	384.06	J/mol×K	810.95	Joback Method
cpg	391.90	J/mol×K	848.52	Joback Method
cpg	399.02	J/mol×K	886.10	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=U357921&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