Carbonic acid, propyl 4-cyanophenyl ester

Inchi: InChI=1S/C11H11NO3/c1-2-7-14-11(13)15-10-5-3-9(8-12)4-6-10/h3-6H,2,7H2,1H3
InchiKey: HNTXLUOVSCFGEY-UHFFFAOYSA-N
Formula: C11H11NO3
SMILES: CCCOC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 205.21

Physical Properties

Property code	Value	Unit	Source
gf	-61.22	kJ/mol	Joback Method
hf	-257.45	kJ/mol	Joback Method
hfus	23.38	kJ/mol	Joback Method
hvap	65.06	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.484		Crippen Method
mcvol	156.780	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1642.00		NIST Webbook
tb	683.53	K	Joback Method
tc	904.98	K	Joback Method
tf	412.05	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.58	J/mol×K	683.53	Joback Method
cpg	405.99	J/mol×K	720.44	Joback Method
cpg	416.64	J/mol×K	757.35	Joback Method
cpg	426.53	J/mol×K	794.25	Joback Method
cpg	435.67	J/mol×K	831.16	Joback Method
cpg	444.04	J/mol×K	868.07	Joback Method
cpg	451.66	J/mol×K	904.98	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=U357821&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