Carbonic acid, allyl 4-cyanophenyl ester

Inchi: InChI=1S/C11H9NO3/c1-2-7-14-11(13)15-10-5-3-9(8-12)4-6-10/h2-6H,1,7H2
InchiKey: GFTAYONHPAZARG-UHFFFAOYSA-N
Formula: C11H9NO3
SMILES: C=CCOC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 203.19

Physical Properties

Property code	Value	Unit	Source
gf	26.62	kJ/mol	Joback Method
hf	-132.02	kJ/mol	Joback Method
hfus	22.10	kJ/mol	Joback Method
hvap	64.39	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.260		Crippen Method
mcvol	152.480	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	680.21	K	Joback Method
tc	905.91	K	Joback Method
tf	410.29	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.79	J/mol×K	680.21	Joback Method
cpg	382.48	J/mol×K	717.83	Joback Method
cpg	392.42	J/mol×K	755.44	Joback Method
cpg	401.63	J/mol×K	793.06	Joback Method
cpg	410.10	J/mol×K	830.68	Joback Method
cpg	417.84	J/mol×K	868.29	Joback Method
cpg	424.86	J/mol×K	905.91	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=U357811&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