Carbonic acid, propyl 4-nitrophenyl ester

Inchi: InChI=1S/C10H11NO5/c1-2-7-15-10(12)16-9-5-3-8(4-6-9)11(13)14/h3-6H,2,7H2,1H3
InchiKey: XQYQGALUIGBFAM-UHFFFAOYSA-N
Formula: C10H11NO5
SMILES: CCCOC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 225.20

Physical Properties

Property code	Value	Unit	Source
gf	-167.27	kJ/mol	Joback Method
hf	-412.45	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.520		Crippen Method
mcvol	158.730	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1763.00		NIST Webbook
tb	710.41	K	Joback Method
tc	944.27	K	Joback Method
tf	479.40	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.11	J/mol×K	710.41	Joback Method
cpg	431.02	J/mol×K	749.39	Joback Method
cpg	442.02	J/mol×K	788.36	Joback Method
cpg	452.10	J/mol×K	827.34	Joback Method
cpg	461.28	J/mol×K	866.31	Joback Method
cpg	469.55	J/mol×K	905.29	Joback Method
cpg	476.93	J/mol×K	944.27	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=U357823&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