Carbonic acid, butyl 4-nitrophenyl ester

Inchi: InChI=1S/C11H13NO5/c1-2-3-8-16-11(13)17-10-6-4-9(5-7-10)12(14)15/h4-7H,2-3,8H2,1
InchiKey: NFLBOYSTEVDVQC-UHFFFAOYSA-N
Formula: C11H13NO5
SMILES: CCCCOC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 239.22

Physical Properties

Property code	Value	Unit	Source
gf	-158.85	kJ/mol	Joback Method
hf	-433.09	kJ/mol	Joback Method
hfus	33.23	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.910		Crippen Method
mcvol	172.820	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook
tb	733.29	K	Joback Method
tc	962.85	K	Joback Method
tf	490.67	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.41	J/mol×K	733.29	Joback Method
cpg	482.86	J/mol×K	771.55	Joback Method
cpg	494.35	J/mol×K	809.81	Joback Method
cpg	504.89	J/mol×K	848.07	Joback Method
cpg	514.48	J/mol×K	886.33	Joback Method
cpg	523.15	J/mol×K	924.59	Joback Method
cpg	530.88	J/mol×K	962.85	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=U357852&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