2-Bromopropionic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C9H8BrNO4/c1-6(10)9(12)15-8-4-2-7(3-5-8)11(13)14/h2-6H,1H3
InchiKey: LOVOFTZGZYJDIM-UHFFFAOYSA-N
Formula: C9H8BrNO4
SMILES: CC(Br)C(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 274.07

Physical Properties

Property code	Value	Unit	Source
gf	-58.81	kJ/mol	Joback Method
hf	-238.54	kJ/mol	Joback Method
hfus	28.63	kJ/mol	Joback Method
hvap	70.36	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.284		Crippen Method
mcvol	156.270	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	1760.00		NIST Webbook
tb	730.83	K	Joback Method
tc	988.84	K	Joback Method
tf	490.70	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.16	J/mol×K	730.83	Joback Method
cpg	386.34	J/mol×K	773.83	Joback Method
cpg	395.59	J/mol×K	816.83	Joback Method
cpg	403.94	J/mol×K	859.84	Joback Method
cpg	411.44	J/mol×K	902.84	Joback Method
cpg	418.12	J/mol×K	945.84	Joback Method
cpg	424.03	J/mol×K	988.84	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=U308027&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