Carbamic acid, 4-bromo-2-nitrophenyl, ethyl ester

Inchi: InChI=1S/C9H9BrN2O4/c1-2-16-9(13)11-7-4-3-6(10)5-8(7)12(14)15/h3-5H,2H2,1H3,(H,1

InchiKey: AUUCTQRLISCVNQ-UHFFFAOYSA-N

Formula: C9H9BrN2O4

SMILES: CCOC(=O)Nc1ccc(Br)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 289.08

Physical Properties

Property code	Value	Unit	Source
gf	23.39	kJ/mol	Joback Method
hf	-191.26	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	77.85	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.926		Crippen Method
mcvol	166.250	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	786.42	K	Joback Method
tc	1036.30	K	Joback Method
tf	570.88	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.03	J/mol×K	786.42	Joback Method
cpg	428.52	J/mol×K	828.07	Joback Method
cpg	437.13	J/mol×K	869.71	Joback Method
cpg	444.89	J/mol×K	911.36	Joback Method
cpg	451.84	J/mol×K	953.01	Joback Method
cpg	458.01	J/mol×K	994.66	Joback Method
cpg	463.43	J/mol×K	1036.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R37795&Units=SI
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

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