Carbamic acid, 4-bromophenyl-, ethyl ester

Inchi: InChI=1S/C9H10BrNO2/c1-2-13-9(12)11-8-5-3-7(10)4-6-8/h3-6H,2H2,1H3,(H,11,12)
InchiKey: ZETBYFYOBYYVOE-UHFFFAOYSA-N
Formula: C9H10BrNO2
SMILES: CCOC(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 244.09

Physical Properties

Property code	Value	Unit	Source
gf	-2.53	kJ/mol	Joback Method
hf	-169.03	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.018		Crippen Method
mcvol	148.830	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	1672.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	629.60	K	Joback Method
tc	859.62	K	Joback Method
tf	414.75	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.82	J/mol×K	629.60	Joback Method
cpg	347.16	J/mol×K	667.94	Joback Method
cpg	357.72	J/mol×K	706.27	Joback Method
cpg	367.53	J/mol×K	744.61	Joback Method
cpg	376.62	J/mol×K	782.95	Joback Method
cpg	384.99	J/mol×K	821.28	Joback Method

cpg	392.70	J/mol×K	859.62	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=U314760&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