Carbamic acid, 2,4-dibromophenyl, ethyl ester

Inchi: InChI=1S/C9H9Br2NO2/c1-2-14-9(13)12-8-4-3-6(10)5-7(8)11/h3-5H,2H2,1H3,(H,12,13)
InchiKey: BEVDUGOXLQDMDS-UHFFFAOYSA-N
Formula: C9H9Br2NO2
SMILES: CCOC(=O)Nc1ccc(Br)cc1Br
Mol. weight [g/mol]: 322.98

Physical Properties

Property code	Value	Unit	Source
gf	2.16	kJ/mol	Joback Method
hf	-154.17	kJ/mol	Joback Method
hfus	30.79	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.780		Crippen Method
mcvol	166.330	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
tb	700.74	K	Joback Method
tc	942.73	K	Joback Method
tf	487.07	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.84	J/mol×K	700.74	Joback Method
cpg	374.71	J/mol×K	741.07	Joback Method
cpg	383.84	J/mol×K	781.40	Joback Method
cpg	392.24	J/mol×K	821.73	Joback Method
cpg	399.95	J/mol×K	862.07	Joback Method
cpg	407.01	J/mol×K	902.40	Joback Method
cpg	413.45	J/mol×K	942.73	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=R37692&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