Carbamic acid, 4-bromophenyl, 1-methylethyl ester

Inchi: InChI=1S/C10H12BrNO2/c1-7(2)14-10(13)12-9-5-3-8(11)4-6-9/h3-7H,1-2H3,(H,12,13)
InchiKey: MGPOTYUNIPGUIA-UHFFFAOYSA-N
Formula: C10H12BrNO2
SMILES: CC(C)OC(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 258.11

Physical Properties

Property code	Value	Unit	Source
gf	3.45	kJ/mol	Joback Method
hf	-194.95	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.406		Crippen Method
mcvol	162.920	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
tb	652.04	K	Joback Method
tc	882.30	K	Joback Method
tf	411.02	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.44	J/mol×K	652.04	Joback Method
cpg	396.83	J/mol×K	690.42	Joback Method
cpg	408.35	J/mol×K	728.79	Joback Method
cpg	419.04	J/mol×K	767.17	Joback Method
cpg	428.93	J/mol×K	805.55	Joback Method
cpg	438.03	J/mol×K	843.93	Joback Method
cpg	446.39	J/mol×K	882.30	Joback Method

Sources

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=R37802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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