Propanamide, N-(4-bromophenyl)-2-chloro-

Inchi: InChI=1S/C9H9BrClNO/c1-6(11)9(13)12-8-4-2-7(10)3-5-8/h2-6H,1H3,(H,12,13)
InchiKey: XUBDXLHGPBQDQM-UHFFFAOYSA-N
Formula: C9H9BrClNO
SMILES: CC(Cl)C(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 262.53

Physical Properties

Property code	Value	Unit	Source
gf	88.10	kJ/mol	Joback Method
hf	-57.83	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	62.18	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.015		Crippen Method
mcvol	155.200	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	1733.00		NIST Webbook
tb	644.17	K	Joback Method
tc	885.79	K	Joback Method
tf	407.44	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.89	J/mol×K	644.17	Joback Method
cpg	346.70	J/mol×K	684.44	Joback Method
cpg	356.65	J/mol×K	724.71	Joback Method
cpg	365.79	J/mol×K	764.98	Joback Method
cpg	374.17	J/mol×K	805.25	Joback Method
cpg	381.86	J/mol×K	845.52	Joback Method
cpg	388.91	J/mol×K	885.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307487&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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