Benzamide, N-(3-chlorophenyl)-3-bromo-

Inchi: InChI=1S/C13H9BrClNO/c14-10-4-1-3-9(7-10)13(17)16-12-6-2-5-11(15)8-12/h1-8H,(H,16
InchiKey: NJSBTVPSISSHNU-UHFFFAOYSA-N
Formula: C13H9BrClNO
SMILES: O=C(Nc1cccc(Cl)c1)c1cccc(Br)c1
Mol. weight [g/mol]: 310.57

Physical Properties

Property code	Value	Unit	Source
gf	227.00	kJ/mol	Joback Method
hf	89.95	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	74.41	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.355		Crippen Method
mcvol	187.800	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	2432.00		NIST Webbook
tb	767.79	K	Joback Method
tc	1030.91	K	Joback Method
tf	506.46	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.57	J/mol×K	767.79	Joback Method
cpg	453.58	J/mol×K	811.64	Joback Method
cpg	463.54	J/mol×K	855.50	Joback Method
cpg	472.54	J/mol×K	899.35	Joback Method
cpg	480.69	J/mol×K	943.20	Joback Method
cpg	488.08	J/mol×K	987.06	Joback Method
cpg	494.80	J/mol×K	1030.91	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=U307154&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