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

Inchi: InChI=1S/C9H9Br2NO/c1-6(10)9(13)12-8-4-2-7(11)3-5-8/h2-6H,1H3,(H,12,13)
InchiKey: FJXNJUQSLIKVOC-UHFFFAOYSA-N
Formula: C9H9Br2NO
SMILES: CC(Br)C(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 306.98

Physical Properties

Property code	Value	Unit	Source
gf	114.35	kJ/mol	Joback Method
hf	-15.76	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	64.23	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.171		Crippen Method
mcvol	160.460	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	1837.00		NIST Webbook
tb	672.90	K	Joback Method
tc	923.18	K	Joback Method
tf	437.32	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.68	J/mol×K	672.90	Joback Method
cpg	355.09	J/mol×K	714.61	Joback Method
cpg	364.62	J/mol×K	756.33	Joback Method
cpg	373.36	J/mol×K	798.04	Joback Method
cpg	381.37	J/mol×K	839.75	Joback Method
cpg	388.72	J/mol×K	881.47	Joback Method
cpg	395.49	J/mol×K	923.18	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=U307477&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