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

Inchi: InChI=1S/C8H7Br2NO/c9-5-8(12)11-7-3-1-6(10)2-4-7/h1-4H,5H2,(H,11,12)
InchiKey: FDPCSKPUJUALLE-UHFFFAOYSA-N
Formula: C8H7Br2NO
SMILES: O=C(CBr)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 292.95

Physical Properties

Property code	Value	Unit	Source
gf	108.37	kJ/mol	Joback Method
hf	10.16	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	62.39	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.783		Crippen Method
mcvol	146.370	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	1826.00		NIST Webbook
tb	650.46	K	Joback Method
tc	901.06	K	Joback Method
tf	441.05	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.87	J/mol×K	650.46	Joback Method
cpg	306.17	J/mol×K	692.23	Joback Method
cpg	314.66	J/mol×K	733.99	Joback Method
cpg	322.43	J/mol×K	775.76	Joback Method
cpg	329.54	J/mol×K	817.53	Joback Method
cpg	336.06	J/mol×K	859.30	Joback Method
cpg	342.05	J/mol×K	901.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307422&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