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

Inchi: InChI=1S/C8H6BrCl2NO/c9-5-1-3-6(4-2-5)12-8(13)7(10)11/h1-4,7H,(H,12,13)
InchiKey: JCMYDJFPADBOJV-UHFFFAOYSA-N
Formula: C8H6BrCl2NO
SMILES: O=C(Nc1ccc(Br)cc1)C(Cl)Cl
Mol. weight [g/mol]: 282.95

Physical Properties

Property code	Value	Unit	Source
gf	67.75	kJ/mol	Joback Method
hf	-52.93	kJ/mol	Joback Method
hfus	26.98	kJ/mol	Joback Method
hvap	64.34	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.191		Crippen Method
mcvol	153.350	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	658.72	K	Joback Method
tc	908.51	K	Joback Method
tf	426.09	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.51	J/mol×K	658.72	Joback Method
cpg	318.43	J/mol×K	700.35	Joback Method
cpg	326.54	J/mol×K	741.98	Joback Method
cpg	333.91	J/mol×K	783.61	Joback Method
cpg	340.60	J/mol×K	825.24	Joback Method
cpg	346.66	J/mol×K	866.88	Joback Method
cpg	352.16	J/mol×K	908.51	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=U307301&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