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

Inchi: InChI=1S/C8H5BrCl3NO/c9-5-1-3-6(4-2-5)13-7(14)8(10,11)12/h1-4H,(H,13,14)
InchiKey: UGJPWLNLVKYGLV-UHFFFAOYSA-N
Formula: C8H5BrCl3NO
SMILES: O=C(Nc1ccc(Br)cc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 317.39

Physical Properties

Property code	Value	Unit	Source
gf	61.10	kJ/mol	Joback Method
hf	-72.14	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	67.82	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.758		Crippen Method
mcvol	165.590	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
rinpol	1892.00		NIST Webbook
tb	693.36	K	Joback Method
tc	955.64	K	Joback Method
tf	473.43	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.21	J/mol×K	693.36	Joback Method
cpg	339.03	J/mol×K	737.07	Joback Method
cpg	345.98	J/mol×K	780.79	Joback Method
cpg	352.19	J/mol×K	824.50	Joback Method
cpg	357.75	J/mol×K	868.22	Joback Method
cpg	362.78	J/mol×K	911.93	Joback Method
cpg	367.39	J/mol×K	955.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307219&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

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