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

Inchi: InChI=1S/C8H7BrClNO/c9-6-1-3-7(4-2-6)11-8(12)5-10/h1-4H,5H2,(H,11,12)
InchiKey: FRZKCMCCQAJIBN-UHFFFAOYSA-N
Formula: C8H7BrClNO
SMILES: O=C(CCl)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 248.50
CAS: 2564-02-5

Physical Properties

Property code	Value	Unit	Source
gf	82.12	kJ/mol	Joback Method
hf	-31.91	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.626		Crippen Method
mcvol	141.110	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
rinpol	1721.00		NIST Webbook
tb	621.73	K	Joback Method
tc	863.34	K	Joback Method
tf	411.17	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.84	J/mol×K	621.73	Joback Method
cpg	298.50	J/mol×K	662.00	Joback Method
cpg	307.39	J/mol×K	702.27	Joback Method
cpg	315.54	J/mol×K	742.53	Joback Method
cpg	323.01	J/mol×K	782.80	Joback Method
cpg	329.85	J/mol×K	823.07	Joback Method
cpg	336.11	J/mol×K	863.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2564025&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