4-Cyclohexyl-2-bromo-acetanilide

Inchi: InChI=1S/C14H18BrNO/c1-10(17)16-14-8-7-12(9-13(14)15)11-5-3-2-4-6-11/h7-9,11H,2-6
InchiKey: MITNMYVLRVDROC-UHFFFAOYSA-N
Formula: C14H18BrNO
SMILES: CC(=O)Nc1ccc(C2CCCCC2)cc1Br
Mol. weight [g/mol]: 296.20
CAS: 5422-53-7

Physical Properties

Property code	Value	Unit	Source
gf	159.39	kJ/mol	Joback Method
hf	-97.16	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	70.40	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.455		Crippen Method
mcvol	202.550	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	746.11	K	Joback Method
tc	994.42	K	Joback Method
tf	468.77	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.95	J/mol×K	746.11	Joback Method
cpg	571.60	J/mol×K	787.50	Joback Method
cpg	586.86	J/mol×K	828.88	Joback Method
cpg	600.84	J/mol×K	870.27	Joback Method
cpg	613.58	J/mol×K	911.65	Joback Method
cpg	625.18	J/mol×K	953.04	Joback Method
cpg	635.71	J/mol×K	994.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5422537&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume