1-(2-Bromo-4-chlorophenoxy)-2-propanol

Inchi: InChI=1S/C9H10BrClO2/c1-6(12)5-13-9-3-2-7(11)4-8(9)10/h2-4,6,12H,5H2,1H3
InchiKey: AAHFKWBQHBFVME-UHFFFAOYSA-N
Formula: C9H10BrClO2
SMILES: CC(O)COc1ccc(Cl)cc1Br
Mol. weight [g/mol]: 265.53
CAS: 116402-66-5

Physical Properties

Property code	Value	Unit	Source
gf	-123.82	kJ/mol	Joback Method
hf	-294.64	kJ/mol	Joback Method
hfus	23.56	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.862		Crippen Method
mcvol	155.390	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	659.71	K	Joback Method
tc	875.11	K	Joback Method
tf	400.42	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.57	J/mol×K	659.71	Joback Method
cpg	387.62	J/mol×K	839.21	Joback Method
cpg	380.33	J/mol×K	803.31	Joback Method
cpg	372.50	J/mol×K	767.41	Joback Method
cpg	364.12	J/mol×K	731.51	Joback Method
cpg	355.15	J/mol×K	695.61	Joback Method
cpg	394.38	J/mol×K	875.11	Joback Method
dvisc	0.0000541	Pa×s	659.71	Joback Method
dvisc	0.0000778	Pa×s	616.50	Joback Method

dvisc	0.0001182	Pa×s	573.28	Joback Method
dvisc	0.0001924	Pa×s	530.07	Joback Method
dvisc	0.0003414	Pa×s	486.85	Joback Method
dvisc	0.0006773	Pa×s	443.63	Joback Method
dvisc	0.0015581	Pa×s	400.42	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=C116402665&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
dvisc:	Dynamic viscosity
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