

2-Bromobenzoic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C13H8BrClO2/c14-12-4-2-1-3-11(12)13(16)17-10-7-5-9(15)6-8-10/h1-8H
InchiKey:	HNHXZDOUQHxDFT-UHFFFAOYSA-N
Formula:	C13H8BrClO2
SMILES:	O=C(Oc1ccc(Cl)cc1)c1ccccc1Br
Mol. weight [g/mol]:	311.56

Physical Properties

Property code	Value	Unit	Source
gf	32.61	kJ/mol	Joback Method
hf	-95.74	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.322		Crippen Method
mvol	183.690	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	740.04	K	Joback Method
tc	1003.05	K	Joback Method
tf	476.03	K	Joback Method
vc	0.682	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.51	J/molxK	740.04	Joback Method
cpg	465.68	J/molxK	959.22	Joback Method
cpg	458.37	J/molxK	915.38	Joback Method
cpg	450.16	J/molxK	871.55	Joback Method
cpg	440.98	J/molxK	827.71	Joback Method
cpg	430.79	J/molxK	783.88	Joback Method
cpg	472.17	J/molxK	1003.05	Joback Method
dvisc	0.0001396	Paxs	740.04	Joback Method

dvisc	0.0001702	Paxs	696.04	Joback Method
dvisc	0.0002132	Paxs	652.04	Joback Method
dvisc	0.0002759	Paxs	608.03	Joback Method
dvisc	0.0003717	Paxs	564.03	Joback Method
dvisc	0.0005267	Paxs	520.03	Joback Method
dvisc	0.0007959	Paxs	476.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U307743&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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