

2-Bromobenzoic acid, 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C13H7BrCl2O2/c14-10-4-2-1-3-9(10)13(17)18-8-5-6-11(15)12(16)7-8/h1-7H
InchiKey:	GZDKZNTZGVTCOJ-UHFFFAOYSA-N
Formula:	C13H7BrCl2O2
SMILES:	O=C(Oc1ccc(Cl)c(Cl)c1)c1ccccc1Br
Mol. weight [g/mol]:	346.00

Physical Properties

Property code	Value	Unit	Source
gf	11.05	kJ/mol	Joback Method
hf	-122.95	kJ/mol	Joback Method
hfus	32.81	kJ/mol	Joback Method
hvap	75.43	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.975		Crippen Method
mcvol	195.930	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpola	2280.00		NIST Webbook
tb	782.45	K	Joback Method
tc	1047.67	K	Joback Method
tf	518.47	K	Joback Method
vc	0.732	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.33	J/molxK	782.45	Joback Method
cpg	447.27	J/molxK	826.65	Joback Method
cpg	456.19	J/molxK	870.86	Joback Method
cpg	464.15	J/molxK	915.06	Joback Method
cpg	471.21	J/molxK	959.26	Joback Method
cpg	477.43	J/molxK	1003.47	Joback Method
cpg	482.86	J/molxK	1047.67	Joback Method
dvisc	0.0006118	Paxs	518.47	Joback Method
dvisc	0.0004232	Paxs	562.47	Joback Method

dvisc	0.0003088	Paxs	606.46	Joback Method
dvisc	0.0002351	Paxs	650.46	Joback Method
dvisc	0.0001853	Paxs	694.46	Joback Method
dvisc	0.0001503	Paxs	738.45	Joback Method
dvisc	0.0001248	Paxs	782.45	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=U307747&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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