

2-Bromobenzoic acid, 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C13H6BrCl3O2/c14-8-4-2-1-3-7(8)13(18)19-12-6-10(16)9(15)5-11(12)17/h1-6H
InchiKey:	HFPASIXJGMHUPY-UHFFFAOYSA-N
Formula:	C13H6BrCl3O2
SMILES:	O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccccc1Br
Mol. weight [g/mol]:	380.45

Physical Properties

Property code	Value	Unit	Source
gf	-10.51	kJ/mol	Joback Method
hf	-150.16	kJ/mol	Joback Method
hfus	36.62	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.629		Crippen Method
mvol	208.170	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	824.86	K	Joback Method
tc	1092.02	K	Joback Method
tf	560.91	K	Joback Method
vc	0.780	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.41	J/molxK	824.86	Joback Method
cpg	462.08	J/molxK	869.39	Joback Method
cpg	469.80	J/molxK	913.91	Joback Method
cpg	476.61	J/molxK	958.44	Joback Method
cpg	482.57	J/molxK	1002.97	Joback Method
cpg	487.72	J/molxK	1047.49	Joback Method
cpg	492.12	J/molxK	1092.02	Joback Method
dvisc	0.0004776	Paxs	560.91	Joback Method

dvisc	0.0003426	Paxs	604.90	Joback Method
dvisc	0.0002570	Paxs	648.89	Joback Method
dvisc	0.0002000	Paxs	692.88	Joback Method
dvisc	0.0001604	Paxs	736.88	Joback Method
dvisc	0.0001318	Paxs	780.87	Joback Method
dvisc	0.0001107	Paxs	824.86	Joback Method

Sources

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=U354679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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