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

Inchi: InChI=1S/C13H6BrCl3O2/c14-8-3-1-2-7(4-8)13(18)19-12-6-10(16)9(15)5-11(12)17/h1-6H

InchiKey: BIDQITLPNYEMGC-UHFFFAOYSA-N

Formula: C13H6BrCl3O2

SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1cccc(Br)c1

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
mcvol	208.170	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
tb	824.86	K	Joback Method
tc	1092.02	K	Joback Method
tf	560.91	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.41	J/mol×K	824.86	Joback Method
cpg	487.72	J/mol×K	1047.49	Joback Method
cpg	482.57	J/mol×K	1002.97	Joback Method
cpg	476.61	J/mol×K	958.44	Joback Method
cpg	469.80	J/mol×K	913.91	Joback Method
cpg	462.08	J/mol×K	869.39	Joback Method
cpg	492.12	J/mol×K	1092.02	Joback Method
dvisc	0.0001107	Pa×s	824.86	Joback Method

dvisc	0.0001318	Pa×s	780.87	Joback Method
dvisc	0.0001604	Pa×s	736.88	Joback Method
dvisc	0.0002000	Pa×s	692.88	Joback Method
dvisc	0.0002570	Pa×s	648.89	Joback Method
dvisc	0.0003426	Pa×s	604.90	Joback Method
dvisc	0.0004776	Pa×s	560.91	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=U355188&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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