2-Bromobenzoic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C9H6BrCl3O2/c10-7-4-2-1-3-6(7)8(14)15-5-9(11,12)13/h1-4H,5H2
InchiKey: VIBXCYRBKKZPAJ-UHFFFAOYSA-N
Formula: C9H6BrCl3O2
SMILES: O=C(OCC(Cl)(Cl)Cl)c1ccccc1Br
Mol. weight [g/mol]: 332.41

Physical Properties

Property code	Value	Unit	Source
gf	-124.87	kJ/mol	Joback Method
hf	-278.47	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	66.02	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.976		Crippen Method
mcvol	175.570	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	1895.00		NIST Webbook
tb	688.49	K	Joback Method
tc	944.11	K	Joback Method
tf	454.27	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.95	J/mol×K	688.49	Joback Method
cpg	366.71	J/mol×K	731.09	Joback Method
cpg	374.60	J/mol×K	773.70	Joback Method
cpg	381.69	J/mol×K	816.30	Joback Method
cpg	388.05	J/mol×K	858.90	Joback Method
cpg	393.77	J/mol×K	901.50	Joback Method
cpg	398.93	J/mol×K	944.11	Joback Method
dvisc	0.0010286	Pa×s	454.27	Joback Method
dvisc	0.0006600	Pa×s	493.31	Joback Method

dvisc	0.0004519	Pa×s	532.34	Joback Method
dvisc	0.0003259	Pa×s	571.38	Joback Method
dvisc	0.0002450	Pa×s	610.42	Joback Method
dvisc	0.0001907	Pa×s	649.45	Joback Method
dvisc	0.0001526	Pa×s	688.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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