

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

Inchi:	InChI=1S/C9H6BrCl3O2/c10-7-3-1-2-6(4-7)8(14)15-5-9(11,12)13/h1-4H,5H2
InchiKey:	RBKLYTYOGNRDII-UHFFFAOYSA-N
Formula:	C9H6BrCl3O2
SMILES:	O=C(OCC(Cl)(Cl)Cl)c1cccc(Br)c1
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	1891.00		NIST Webbook
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tb	688.49	K	Joback Method
tc	944.11	K	Joback Method
tf	454.27	K	Joback Method
vc	0.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.95	J/molxK	688.49	Joback Method
cpg	366.71	J/molxK	731.09	Joback Method
cpg	374.60	J/molxK	773.70	Joback Method
cpg	381.69	J/molxK	816.30	Joback Method
cpg	388.05	J/molxK	858.90	Joback Method
cpg	393.77	J/molxK	901.50	Joback Method
cpg	398.93	J/molxK	944.11	Joback Method
dvisc	0.0010286	Paxs	454.27	Joback Method

dvisc	0.0006600	Paxs	493.31	Joback Method
dvisc	0.0004519	Paxs	532.34	Joback Method
dvisc	0.0003259	Paxs	571.38	Joback Method
dvisc	0.0002450	Paxs	610.42	Joback Method
dvisc	0.0001907	Paxs	649.45	Joback Method
dvisc	0.0001526	Paxs	688.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355184&Units=SI
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

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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