

3-Bromobenzoic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C10H8BrClO2/c11-9-4-1-3-8(7-9)10(13)14-6-2-5-12/h1-5,7H,6H2/b5-2+
InchiKey:	MFKOGTUUCZQPKL-GORDUTHDSA-N
Formula:	C10H8BrClO2
SMILES:	O=C(OCC=CCl)c1cccc(Br)c1
Mol. weight [g/mol]:	275.53

Physical Properties

Property code	Value	Unit	Source
gf	-15.21	kJ/mol	Joback Method
hf	-141.66	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.358		Crippen Method
mvol	160.880	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	643.90	K	Joback Method
tc	884.33	K	Joback Method
tf	398.20	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.32	J/molxK	643.90	Joback Method
cpg	383.56	J/molxK	844.26	Joback Method
cpg	375.93	J/molxK	804.19	Joback Method
cpg	367.64	J/molxK	764.12	Joback Method
cpg	358.65	J/molxK	724.04	Joback Method
cpg	348.89	J/molxK	683.97	Joback Method
cpg	390.58	J/molxK	884.33	Joback Method
dvisc	0.0001703	Paxs	643.90	Joback Method

dvisc	0.0002110	Paxs	602.95	Joback Method
dvisc	0.0002699	Paxs	562.00	Joback Method
dvisc	0.0003587	Paxs	521.05	Joback Method
dvisc	0.0005005	Paxs	480.10	Joback Method
dvisc	0.0007430	Paxs	439.15	Joback Method
dvisc	0.0011966	Paxs	398.20	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=U299149&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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