

Methyl 3-bromo-2,2-dichloro-propanoate

Inchi:	InChI=1S/C4H5BrCl2O2/c1-9-3(8)4(6,7)2-5/h2H2,1H3
InchiKey:	AUHZFXMFSGANDP-UHFFFAOYSA-N
Formula:	C4H5BrCl2O2
SMILES:	COC(=O)C(Cl)(Cl)CBr
Mol. weight [g/mol]:	235.89
CAS:	89294-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-257.82	kJ/mol	Joback Method
hf	-384.59	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	47.56	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.728		Crippen Method
mcvol	116.640	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	505.00	K	Joback Method
tc	730.08	K	Joback Method
tf	329.06	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.73	J/molxK	505.00	Joback Method
cpg	232.38	J/molxK	692.57	Joback Method
cpg	227.40	J/molxK	655.06	Joback Method
cpg	221.98	J/molxK	617.54	Joback Method
cpg	216.08	J/molxK	580.03	Joback Method
cpg	209.68	J/molxK	542.51	Joback Method
cpg	236.94	J/molxK	730.08	Joback Method
dvisc	0.0003551	Paxs	505.00	Joback Method
dvisc	0.0004491	Paxs	475.68	Joback Method

dvisc	0.0005857	Paxs	446.35	Joback Method
dvisc	0.0007930	Paxs	417.03	Joback Method
dvisc	0.0011240	Paxs	387.71	Joback Method
dvisc	0.0016867	Paxs	358.38	Joback Method
dvisc	0.0027211	Paxs	329.06	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=C89294735&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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