

Bromoacetic acid, 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C8H5BrCl2O2/c9-4-8(12)13-5-1-2-6(10)7(11)3-5/h1-3H,4H2
InchiKey:	BWDIBLSMEKLSNP-UHFFFAOYSA-N
Formula:	C8H5BrCl2O2
SMILES:	O=C(CBr)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	283.93

Physical Properties

Property code	Value	Unit	Source
gf	-133.83	kJ/mol	Joback Method
hf	-244.81	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.294		Crippen Method
mcvol	149.240	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
rinpol	1683.00		NIST Webbook
tb	636.39	K	Joback Method
tc	880.75	K	Joback Method
tf	423.18	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.70	J/molxK	636.39	Joback Method
cpg	295.10	J/molxK	677.12	Joback Method
cpg	302.86	J/molxK	717.84	Joback Method
cpg	310.00	J/molxK	758.57	Joback Method
cpg	316.54	J/molxK	799.29	Joback Method
cpg	322.49	J/molxK	840.02	Joback Method
cpg	327.87	J/molxK	880.75	Joback Method
dvisc	0.0010906	Paxs	423.18	Joback Method
dvisc	0.0007576	Paxs	458.72	Joback Method

dvisc	0.0005546	Paxs	494.25	Joback Method
dvisc	0.0004233	Paxs	529.78	Joback Method
dvisc	0.0003343	Paxs	565.32	Joback Method
dvisc	0.0002714	Paxs	600.86	Joback Method
dvisc	0.0002256	Paxs	636.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308050&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

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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