

2-Bromopropionic acid, 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C9H7BrCl2O2/c1-5(10)9(13)14-6-2-3-7(11)8(12)4-6/h2-5H,1H3
InchiKey:	HOKTYFOLCUZQDD-UHFFFAOYSA-N
Formula:	C9H7BrCl2O2
SMILES:	CC(Br)C(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	297.96

Physical Properties

Property code	Value	Unit	Source
gf	-127.85	kJ/mol	Joback Method
hf	-270.73	kJ/mol	Joback Method
hfus	25.27	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.682		Crippen Method
mcvol	163.330	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinqol	1698.00		NIST Webbook
tb	658.83	K	Joback Method
tc	903.07	K	Joback Method
tf	419.45	K	Joback Method
vc	0.610	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.57	J/molxK	658.83	Joback Method
cpg	343.18	J/molxK	699.54	Joback Method
cpg	352.04	J/molxK	740.24	Joback Method
cpg	360.19	J/molxK	780.95	Joback Method
cpg	367.64	J/molxK	821.66	Joback Method
cpg	374.42	J/molxK	862.36	Joback Method
cpg	380.56	J/molxK	903.07	Joback Method
dvisc	0.0011717	Paxs	419.45	Joback Method
dvisc	0.0007550	Paxs	459.35	Joback Method

dvisc	0.0005219	Paxs	499.24	Joback Method
dvisc	0.0003811	Paxs	539.14	Joback Method
dvisc	0.0002905	Paxs	579.04	Joback Method
dvisc	0.0002294	Paxs	618.93	Joback Method
dvisc	0.0001864	Paxs	658.83	Joback Method

Sources

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=U308026&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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