

Benzoic acid, 5-bromo-2-chloro-, ethyl ester

Other names:	ethyl 5-bromo-2-chlorobenzoate
Inchi:	InChI=1S/C9H8BrClO2/c1-2-13-9(12)7-5-6(10)3-4-8(7)11/h3-5H,2H2,1H3
InchiKey:	AMGWDYLEMSUIO-UHFFFAOYSA-N
Formula:	C9H8BrClO2
SMILES:	CCOC(=O)c1cc(Br)ccc1Cl
Mol. weight [g/mol]:	263.52
CAS:	76008-73-6

Physical Properties

Property code	Value	Unit	Source
gf	-113.48	kJ/mol	Joback Method
hf	-249.71	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	59.20	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.279		Crippen Method
mcvol	151.090	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
tb	621.84	K	Joback Method
tc	858.00	K	Joback Method
tf	404.53	K	Joback Method
vc	0.567	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.15	J/molxK	621.84	Joback Method
cpg	322.40	J/molxK	661.20	Joback Method
cpg	331.96	J/molxK	700.56	Joback Method
cpg	340.85	J/molxK	739.92	Joback Method
cpg	349.07	J/molxK	779.28	Joback Method
cpg	356.66	J/molxK	818.64	Joback Method
cpg	363.63	J/molxK	858.00	Joback Method
dvisc	0.0011425	Paxs	404.53	Joback Method

dvisc	0.0007746	Paxs	440.75	Joback Method
dvisc	0.0005571	Paxs	476.97	Joback Method
dvisc	0.0004197	Paxs	513.19	Joback Method
dvisc	0.0003283	Paxs	549.40	Joback Method
dvisc	0.0002647	Paxs	585.62	Joback Method
dvisc	0.0002188	Paxs	621.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76008736&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

cp_g:	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:	Log ₁₀ 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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