Ethyl 2-bromobenzoate

Other names: Benzoic acid, 2-bromo-, ethyl ester
2-Bromobezoic acid, ethyl ester
Inchi: InChI=1S/C9H9BrO2/c1-2-12-9(11)7-5-3-4-6-8(7)10/h3-6H,2H2,1H3
InchiKey: BIHHBTVQFPVSTE-UHFFFAOYSA-N
Formula: C9H9BrO2
SMILES: CCOC(=O)c1ccccc1Br
Mol. weight [g/mol]: 229.07
CAS: 6091-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-91.92	kJ/mol	Joback Method
hf	-222.50	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.626		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	527.70	K	NIST Webbook
tb	527.50 ± 0.50	K	NIST Webbook
tc	811.07	K	Joback Method
tf	362.09	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.08	J/mol×K	579.43	Joback Method
cpg	302.44	J/mol×K	618.04	Joback Method
cpg	313.06	J/mol×K	656.64	Joback Method
cpg	322.96	J/mol×K	695.25	Joback Method
cpg	332.17	J/mol×K	733.85	Joback Method
cpg	340.71	J/mol×K	772.46	Joback Method

cpg	348.60	J/mol×K	811.07	Joback Method
dvisc	0.0015157	Pa×s	362.09	Joback Method
dvisc	0.0009661	Pa×s	398.31	Joback Method
dvisc	0.0006638	Pa×s	434.54	Joback Method
dvisc	0.0004832	Pa×s	470.76	Joback Method
dvisc	0.0003681	Pa×s	506.98	Joback Method
dvisc	0.0002908	Pa×s	543.21	Joback Method
dvisc	0.0002365	Pa×s	579.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.20	K	2.30	NIST Webbook
tbrp	390.00	K	2.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C6091641&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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