3-Bromobenzoic acid, ethyl ester

Other names:	Benzoic acid, m-bromo-, ethyl ester
	Ethyl 3-bromobenzoate
	3-Bromobenzoic acid, ethyl ester
Inchi:	InChI=1S/C9H9BrO2/c1-2-12-9(11)7-4-3-5-8(10)6-7/h3-6H,2H2,1H3
InchiKey:	QAUASTLEZAPQTB-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	CCOC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	229.07

Physical Properties

Property code	Value	Unit	Source
af	0.5077		Cheméo Relay (1.0)
hf	-296.53	kJ/mol	Cheméo Relay (1.0)
hfus	20.79	kJ/mol	Joback Method
hvap	69.05	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-3.76		Cheméo Relay (1.0)
logp	2.626		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	534.00	K	NIST Webbook
tb	534.20	K	NIST Webbook
tc	737.01	K	Cheméo Relay (1.0)
tf	278.16	K	Cheméo Relay (1.0)
vc	0.497	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.08	J/mol×K	579.43	Joback Method
cpg	348.60	J/mol×K	811.07	Joback Method
cpg	340.71	J/mol×K	772.46	Joback Method
cpg	332.17	J/mol×K	733.85	Joback Method
cpg	322.96	J/mol×K	695.25	Joback Method

cpg	313.06	J/mol×K	656.64	Joback Method
cpg	302.44	J/mol×K	618.04	Joback Method
dvisc	0.0004832	Pa×s	470.76	Joback Method
dvisc	0.0002365	Pa×s	579.43	Joback Method
dvisc	0.0002908	Pa×s	543.21	Joback Method
dvisc	0.0003681	Pa×s	506.98	Joback Method
dvisc	0.0015157	Pa×s	362.09	Joback Method
dvisc	0.0006638	Pa×s	434.54	Joback Method
dvisc	0.0009661	Pa×s	398.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.70	K	1.60	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24398887&Units=SI

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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