Ethanol, 2-bromo-

Other names:	Ethylene bromohydrin
	Glycol bromohydrin
	1-Bromo-2-ethanol
	2-Bromoethanol
	2-Hydroxyethyl bromide
	CH2BrCH2OH(trans)
Inchi:	InChI=1S/C2H5BrO/c3-1-2-4/h4H,1-2H2
InchiKey:	LDLCZOVUSADOIV-UHFFFAOYSA-N
Formula:	C2H5BrO
SMILES:	OCCBr
Mol. weight [g/mol]:	124.96
CAS:	540-51-2

Physical Properties

Property code	Value	Unit	Source
affp	766.10	kJ/mol	NIST Webbook
basg	735.70	kJ/mol	NIST Webbook
gf	-156.54	kJ/mol	Joback Method
hf	-210.51	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	54.10 ± 0.40	kJ/mol	NIST Webbook
ie	10.57	eV	NIST Webbook
ie	10.65	eV	NIST Webbook
ie	10.75	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
ie	10.63	eV	NIST Webbook
ie	10.63	eV	NIST Webbook
ie	10.62	eV	NIST Webbook
log10ws	-0.35		Crippen Method
logp	0.374		Crippen Method
mcvol	62.410	ml/mol	McGowan Method
pc	6410.25	kPa	Joback Method
ripol	1492.00		NIST Webbook
ripol	1492.00		NIST Webbook
tb	423.40 ± 0.70	K	NIST Webbook
tc	585.51	K	Joback Method

tf	232.92	K	Joback Method
vc	0.229	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	95.18	J/mol×K	403.50	Joback Method
cpg	114.32	J/mol×K	555.17	Joback Method
cpg	110.87	J/mol×K	524.84	Joback Method
cpg	107.24	J/mol×K	494.50	Joback Method
cpg	103.42	J/mol×K	464.17	Joback Method
cpg	99.41	J/mol×K	433.83	Joback Method
cpg	117.60	J/mol×K	585.51	Joback Method
dvisc	0.0004697	Pa×s	403.50	Joback Method
dvisc	0.0007517	Pa×s	375.07	Joback Method
dvisc	0.0012994	Pa×s	346.64	Joback Method
dvisc	0.0024771	Pa×s	318.21	Joback Method
dvisc	0.0053593	Pa×s	289.78	Joback Method
dvisc	0.0137149	Pa×s	261.35	Joback Method
dvisc	0.0441470	Pa×s	232.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	329.70	K	2.70	NIST Webbook

Sources

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=C540512&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume