

Ethane, 1-bromo-2-methoxy-

Other names:	2-Bromoethyl methyl ether 1-Bromo-2-methoxyethane Ether, 2-bromoethyl methyl Methoxyethyl bromide 2-Methoxyethyl bromide
Inchi:	InChI=1S/C3H7BrO/c1-5-3-2-4/h2-3H2,1H3
InchiKey:	YZUPZGFPHUVJKC-UHFFFAOYSA-N
Formula:	C3H7BrO
SMILES:	COCCBr
Mol. weight [g/mol]:	138.99
CAS:	6482-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-116.30	kJ/mol	Joback Method
hf	-211.14	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	31.12	kJ/mol	Joback Method
ie	10.13	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	1.028		Crippen Method
mcvol	76.500	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpola	696.00		NIST Webbook
rinpola	716.20		NIST Webbook
rinpola	716.20		NIST Webbook
rinpola	696.00		NIST Webbook
tb	383.00 ± 1.00	K	NIST Webbook
tc	543.29	K	Joback Method
tf	205.60	K	Joback Method
vc	0.283	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.42	J/molxK	356.62	Joback Method
cpg	121.36	J/molxK	387.73	Joback Method
cpg	127.12	J/molxK	418.84	Joback Method
cpg	132.70	J/molxK	449.96	Joback Method
cpg	138.09	J/molxK	481.07	Joback Method
cpg	143.31	J/molxK	512.18	Joback Method
cpg	148.34	J/molxK	543.29	Joback Method
dvisc	0.0026168	Paxs	205.60	Joback Method
dvisc	0.0015397	Paxs	230.77	Joback Method
dvisc	0.0010055	Paxs	255.94	Joback Method
dvisc	0.0007088	Paxs	281.11	Joback Method
dvisc	0.0005291	Paxs	306.28	Joback Method
dvisc	0.0004130	Paxs	331.45	Joback Method
dvisc	0.0003338	Paxs	356.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	313.70	K	8.80	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=C6482242&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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