BROMOMETHYL METHYL ETHER

Other names: Ether, bromomethyl methyl
Methane, bromomethoxy-
Methoxymethyl bromide
Inchi: InChI=1S/C2H5BrO/c1-4-2-3/h2H2,1H3
InchiKey: JAMFGQBENKSWOF-UHFFFAOYSA-N
Formula: C2H5BrO
SMILES: COCBr
Mol. weight [g/mol]: 124.96

Physical Properties

Property code	Value	Unit	Source
af	0.3323		Cheméo Relay (1.0)
gf	-124.72	kJ/mol	Joback Method
hf	-167.15	kJ/mol	Cheméo Relay (1.0)
hfus	7.41	kJ/mol	Joback Method
hvap	30.95	kJ/mol	Cheméo Relay (1.0)
ie	10.15	eV	Cheméo Relay (1.0)
log10ws	-0.38		Cheméo Relay (1.0)
logp	0.985		Crippen Method
mcvol	62.410	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	360.20	K	NIST Webbook
tc	532.01	K	Cheméo Relay (1.0)
tf	187.25	K	Cheméo Relay (1.0)
vc	0.225	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.75	J/mol×K	333.74	Joback Method
cpg	89.93	J/mol×K	364.90	Joback Method
cpg	94.00	J/mol×K	396.07	Joback Method
cpg	97.97	J/mol×K	427.23	Joback Method
cpg	101.83	J/mol×K	458.40	Joback Method

cpg	105.58	J/mol×K	489.56	Joback Method
cpg	109.22	J/mol×K	520.73	Joback Method
dvisc	0.0023445	Pa×s	194.33	Joback Method
dvisc	0.0014253	Pa×s	217.56	Joback Method
dvisc	0.0009538	Pa×s	240.80	Joback Method
dvisc	0.0006851	Pa×s	264.03	Joback Method
dvisc	0.0005191	Pa×s	287.27	Joback Method
dvisc	0.0004100	Pa×s	310.50	Joback Method
dvisc	0.0003347	Pa×s	333.74	Joback Method

Sources

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=C13057175&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume