

2-Butoxyethyl bromide

Other names:	2-(n-Butoxy)ethyl bromide Butane, 1-(2-bromoethoxy)- Ether, 2-bromoethyl butyl 2-Bromoethyl butyl ether
Inchi:	InChI=1S/C6H13BrO/c1-2-3-5-8-6-4-7/h2-6H2,1H3
InchiKey:	WOLUYEFMPZAHNN-UHFFFAOYSA-N
Formula:	C6H13BrO
SMILES:	CCCCOCCBr
Mol. weight [g/mol]:	181.07
CAS:	6550-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-91.04	kJ/mol	Joback Method
hf	-273.06	kJ/mol	Joback Method
hfus	17.77	kJ/mol	Joback Method
hvap	37.80	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	2.198		Crippen Method
mcvol	118.770	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	425.26	K	Joback Method
tc	608.72	K	Joback Method
tf	239.41	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.99	J/mol×K	425.26	Joback Method
cpg	230.39	J/mol×K	455.84	Joback Method
cpg	240.40	J/mol×K	486.41	Joback Method
cpg	250.02	J/mol×K	516.99	Joback Method
cpg	259.27	J/mol×K	547.57	Joback Method

cpg	268.15	J/mol×K	578.15	Joback Method
cpg	276.66	J/mol×K	608.72	Joback Method
dvisc	0.0030729	Pa×s	239.41	Joback Method
dvisc	0.0016637	Pa×s	270.38	Joback Method
dvisc	0.0010218	Pa×s	301.36	Joback Method
dvisc	0.0006873	Pa×s	332.33	Joback Method
dvisc	0.0004946	Pa×s	363.31	Joback Method
dvisc	0.0003749	Pa×s	394.28	Joback Method
dvisc	0.0002958	Pa×s	425.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.50 ± 0.50	K	1.70	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=C6550998&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
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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