1,4-bromoethoxybutane

Other names: Butane, 1-bromo-4-ethoxy
Inchi: InChI=1S/C6H13BrO/c1-2-8-6-4-3-5-7/h2-6H2,1H3
InchiKey: AABRBNAXKRILNN-UHFFFAOYSA-N
Formula: C6H13BrO
SMILES: CCOCCCCBr
Mol. weight [g/mol]: 181.07

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
rinpol	994.30		NIST Webbook
rinpol	1001.30		NIST Webbook
rinpol	994.30		NIST Webbook
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

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=R135805&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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