

Propane, 1-bromo-3-ethoxy-

Other names:	3-ethoxypropyl bromide
Inchi:	InChI=1S/C5H11BrO/c1-2-7-5-3-4-6/h2-5H2,1H3
InchiKey:	JOZWPJGRGUOZGY-UHFFFAOYSA-N
Formula:	C5H11BrO
SMILES:	CCOCCCCBr
Mol. weight [g/mol]:	167.04
CAS:	36865-40-4

Physical Properties

Property code	Value	Unit	Source
gf	-99.46	kJ/mol	Joback Method
hf	-252.42	kJ/mol	Joback Method
hfus	15.18	kJ/mol	Joback Method
hvap	35.57	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.808		Crippen Method
mcvol	104.680	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	890.80		NIST Webbook
rinpol	880.80		NIST Webbook
tb	421.65 ± 2.50	K	NIST Webbook
tc	587.20	K	Joback Method
tf	228.14	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.67	J/mol×K	402.38	Joback Method
cpg	224.71	J/mol×K	556.39	Joback Method
cpg	216.94	J/mol×K	525.59	Joback Method
cpg	208.85	J/mol×K	494.79	Joback Method
cpg	200.45	J/mol×K	463.99	Joback Method
cpg	191.72	J/mol×K	433.18	Joback Method

cpg	232.18	J/mol×K	587.20	Joback Method
dvisc	0.0003128	Pa×s	402.38	Joback Method
dvisc	0.0003935	Pa×s	373.34	Joback Method
dvisc	0.0005147	Pa×s	344.30	Joback Method
dvisc	0.0007073	Pa×s	315.26	Joback Method
dvisc	0.0010367	Pa×s	286.22	Joback Method
dvisc	0.0016566	Pa×s	257.18	Joback Method
dvisc	0.0029827	Pa×s	228.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36865404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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