Oxirane, (bromomethyl)-

Other names:	Propane, 1-bromo-2,3-epoxy-
	(Bromomethyl)ethylene oxide
	Epibromhydrin
	Epibromohydrin
	1-Bromo-2,3-epoxypropane
	1,2-Epoxy-3-bromopropane
	2-(Bromomethyl)oxirane
	(Bromomethyl)oxirane
	Epibromohydrine
	Propane, 3-bromo-1,2-epoxy-
	3-Bromo-1,2-epoxypropane
	UN 2558
	(.+/-.)-(Bromomethyl)oxirane
	NSC 630
	Oxirane, 2-(bromomethyl)-
Inchi:	InChI=1S/C3H5BrO/c4-1-3-2-5-3/h3H,1-2H2
InchiKey:	GKIPXFAANLTWBM-UHFFFAOYSA-N
Formula:	C3H5BrO
SMILES:	BrCC1CO1
Mol. weight [g/mol]:	136.97
CAS:	3132-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-36.67	kJ/mol	Joback Method
hf	-138.12	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	33.13	kJ/mol	Joback Method
ie	10.46	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.780		Crippen Method
mcvol	65.640	ml/mol	McGowan Method
pc	5774.15	kPa	Joback Method
rinpol	805.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	773.00		NIST Webbook

ripol	1330.00		NIST Webbook
tb	412.50 ± 0.50	K	NIST Webbook
tb	408.20	K	NIST Webbook
tc	573.19	K	Joback Method
tf	227.88	K	Joback Method
vc	0.243	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.12	J/mol×K	367.89	Joback Method
cpg	133.58	J/mol×K	538.97	Joback Method
cpg	128.06	J/mol×K	504.76	Joback Method
cpg	122.08	J/mol×K	470.54	Joback Method
cpg	115.63	J/mol×K	436.32	Joback Method
cpg	108.65	J/mol×K	402.11	Joback Method
cpg	138.70	J/mol×K	573.19	Joback Method
dvisc	0.0005998	Pa×s	367.89	Joback Method
dvisc	0.0006685	Pa×s	344.55	Joback Method
dvisc	0.0007568	Pa×s	321.22	Joback Method
dvisc	0.0008737	Pa×s	297.88	Joback Method
dvisc	0.0010335	Pa×s	274.55	Joback Method
dvisc	0.0012612	Pa×s	251.22	Joback Method
dvisc	0.0016033	Pa×s	227.88	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3132647&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume