

Isobutylene epoxide

Other names:	1,1-Dimethylethylene oxide 1,2-Epoxyisobutane 1,2-Isobutylene oxide 1,2-epoxy-2-methylpropane 2,2-dimethyloxirane 2-Methyl-1-propene oxide 2-methyl-1,2-epoxypropane Isobutene oxide NSC 24249 Propane, 1,2-epoxy-2-methyl- isobutylene oxide oxirane, 2,2-dimethyl-
Inchi:	InChI=1S/C4H8O/c1-4(2)3-5-4/h3H2,1-2H3
InchiKey:	GELKGHVAFRCJNA-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	CC1(C)CO1
Mol. weight [g/mol]:	72.11
CAS:	558-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-48.06	kJ/mol	Joback Method
hf	-169.85	kJ/mol	Joback Method
hfus	5.93	kJ/mol	Joback Method
hvap	27.77	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.795		Crippen Method
mcvol	62.230	ml/mol	McGowan Method
pc	4350.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
rinpol	535.00		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	510.00		NIST Webbook

rinpol	500.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	534.40		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	534.40		NIST Webbook
rinpol	534.70		NIST Webbook
tb	325.00	K	NIST Webbook
tb	347.65 ± 5.00	K	NIST Webbook
tb	325.15 ± 3.00	K	NIST Webbook
tb	324.65 ± 2.00	K	NIST Webbook
tb	323.15 ± 1.50	K	NIST Webbook
tb	325.20	K	NIST Webbook
tc	514.29	K	Joback Method
tf	207.00 ± 0.60	K	NIST Webbook
vc	0.235	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.04	J/mol×K	324.85	Joback Method
cpg	110.66	J/mol×K	356.42	Joback Method
cpg	120.32	J/mol×K	388.00	Joback Method
cpg	129.11	J/mol×K	419.57	Joback Method
cpg	137.11	J/mol×K	451.14	Joback Method
cpg	144.40	J/mol×K	482.72	Joback Method
cpg	151.05	J/mol×K	514.29	Joback Method
hvapt	30.60	kJ/mol	266.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C558305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Effect of anion species on infinite dilution activity coefficients of organic compounds in aqueous solution	https://www.doi.org/10.1016/j.fluid.2010.01.007
Spontaneous emulsification pressure measurements for 17 Compounds by a Low Pressure Time Flow Method:	https://www.doi.org/10.1021/je060269j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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