

2,2'-Bioxirane, (2S,2'S)-

Other names:	(2S,2'S)-2,2'-Bioxirane (2s,3s)-Diepoxybutane
Inchi:	InChI=1S/C4H6O2/c1-3(5-1)4-2-6-4/h3-4H,1-2H2/t3-,4-/m1/s1
InchiKey:	ZFIVKAOQEXOYFY-QWWZWVQMSA-N
Formula:	C4H6O2
SMILES:	C1OC1C1CO1
Mol. weight [g/mol]:	86.09
CAS:	30031-64-2

Physical Properties

Property code	Value	Unit	Source
gf	-67.94	kJ/mol	Joback Method
hf	-244.29	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	33.34	kJ/mol	Joback Method
log10ws	0.32		Crippen Method
logp	-0.216		Crippen Method
mvol	57.240	ml/mol	McGowan Method
pc	5406.57	kPa	Joback Method
tb	417.80 ± 0.20	K	NIST Webbook
tc	558.39	K	Joback Method
tf	297.85 ± 0.85	K	NIST Webbook
vc	0.215	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	109.07	J/mol×K	358.30	Joback Method
cpg	154.56	J/mol×K	525.04	Joback Method
cpg	146.83	J/mol×K	491.69	Joback Method
cpg	138.46	J/mol×K	458.35	Joback Method
cpg	129.41	J/mol×K	425.00	Joback Method
cpg	119.63	J/mol×K	391.65	Joback Method
cpg	161.70	J/mol×K	558.39	Joback Method

dvisc	0.0005861	Paxs	358.30	Joback Method
dvisc	0.0005981	Paxs	335.89	Joback Method
dvisc	0.0006122	Paxs	313.49	Joback Method
dvisc	0.0006288	Paxs	291.08	Joback Method
dvisc	0.0006488	Paxs	268.67	Joback Method
dvisc	0.0006732	Paxs	246.27	Joback Method
dvisc	0.0007038	Paxs	223.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.00	K	6.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C30031642&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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