

2-Butanol, 3,3'-oxybis-

Other names:	3,3'-Oxybis(butan-2-ol)
Inchi:	InChI=1S/C8H18O3/c1-5(9)7(3)11-8(4)6(2)10/h5-10H,1-4H3
InchiKey:	GWHZXOQHXAXFQK-UHFFFAOYSA-N
Formula:	C8H18O3
SMILES:	CC(O)C(C)OC(C)C(C)O
Mol. weight [g/mol]:	162.23
CAS:	54305-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-371.92	kJ/mol	Joback Method
hf	-666.25	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	67.62	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.542		Crippen Method
mcvol	141.190	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1112.30		NIST Webbook
rinpol	1112.30		NIST Webbook
tb	587.46	K	Joback Method
tc	754.52	K	Joback Method
tf	263.79	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.82	J/molxK	587.46	Joback Method
cpg	421.17	J/molxK	726.68	Joback Method
cpg	411.96	J/molxK	698.83	Joback Method
cpg	402.34	J/molxK	670.99	Joback Method
cpg	392.27	J/molxK	643.15	Joback Method
cpg	381.77	J/molxK	615.30	Joback Method

cpg	429.95	J/molxK	754.52	Joback Method
dvisc	0.0000247	Paxs	587.46	Joback Method
dvisc	0.0000561	Paxs	533.52	Joback Method
dvisc	0.0001535	Paxs	479.57	Joback Method
dvisc	0.0005426	Paxs	425.62	Joback Method
dvisc	0.0027656	Paxs	371.68	Joback Method
dvisc	0.0245082	Paxs	317.74	Joback Method
dvisc	0.5301176	Paxs	263.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54305612&Units=SI
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

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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