

Butane, 2,2'-[methylenebis(oxy)]bis-

Other names:	Methane, di-sec-butoxy- Di-(2-butoxy)methane Methane, di-(2-butyloxy)
Inchi:	InChI=1S/C9H20O2/c1-5-8(3)10-7-11-9(4)6-2/h8-9H,5-7H2,1-4H3
InchiKey:	YJBUXLCNFPNEB-UHFFFAOYSA-N
Formula:	C9H20O2
SMILES:	CCC(C)OCOC(C)CC
Mol. weight [g/mol]:	160.25
CAS:	2568-92-5

Physical Properties

Property code	Value	Unit	Source
gf	-189.98	kJ/mol	Joback Method
hf	-504.09	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	39.67	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.574		Crippen Method
mcvol	149.410	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	946.00		NIST Webbook
rinpol	952.00		NIST Webbook
tb	449.28	K	Joback Method
tc	619.70	K	Joback Method
tf	205.65	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.90	J/mol×K	449.28	Joback Method
cpg	339.18	J/mol×K	477.68	Joback Method
cpg	353.03	J/mol×K	506.09	Joback Method
cpg	366.43	J/mol×K	534.49	Joback Method

cpg	379.40	J/mol×K	562.89	Joback Method
cpg	391.92	J/mol×K	591.30	Joback Method
cpg	403.99	J/mol×K	619.70	Joback Method
dvisc	0.0081421	Pa×s	205.65	Joback Method
dvisc	0.0024899	Pa×s	246.25	Joback Method
dvisc	0.0010648	Pa×s	286.86	Joback Method
dvisc	0.0005622	Pa×s	327.47	Joback Method
dvisc	0.0003417	Pa×s	368.07	Joback Method
dvisc	0.0002293	Pa×s	408.67	Joback Method
dvisc	0.0001654	Pa×s	449.28	Joback Method

Sources

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=C2568925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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