

Butane, 1,4-dimethoxy-

Other names:	1,4-Dimethoxybutane CH3O(CH2)4OCH3
Inchi:	InChI=1S/C6H14O2/c1-7-5-3-4-6-8-2/h3-6H2,1-2H3
InchiKey:	HMCUNLUHTBHKTB-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	COCCCCOC
Mol. weight [g/mol]:	118.17
CAS:	13179-96-9

Physical Properties

Property code	Value	Unit	Source
affp	931.50	kJ/mol	NIST Webbook
basg	880.60	kJ/mol	NIST Webbook
gf	-210.36	kJ/mol	Joback Method
hf	-431.61	kJ/mol	Joback Method
hfus	13.67	kJ/mol	Joback Method
hvap	33.77	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	1.059		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	806.60		NIST Webbook
rinpol	807.70		NIST Webbook
rinpol	806.60		NIST Webbook
rinpol	855.00		NIST Webbook
tb	381.52	K	Joback Method
tc	546.82	K	Joback Method
tf	201.84	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.67	J/mol×K	381.52	Joback Method

cpg	214.60	J/mol×K	409.07	Joback Method
cpg	224.32	J/mol×K	436.62	Joback Method
cpg	233.82	J/mol×K	464.17	Joback Method
cpg	243.09	J/mol×K	491.72	Joback Method
cpg	252.13	J/mol×K	519.27	Joback Method
cpg	260.92	J/mol×K	546.82	Joback Method
dvisc	0.0027699	Pa×s	201.84	Joback Method
dvisc	0.0013528	Pa×s	231.79	Joback Method
dvisc	0.0007784	Pa×s	261.73	Joback Method
dvisc	0.0005017	Pa×s	291.68	Joback Method
dvisc	0.0003510	Pa×s	321.63	Joback Method
dvisc	0.0002609	Pa×s	351.57	Joback Method
dvisc	0.0002032	Pa×s	381.52	Joback Method

Sources

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=C13179969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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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