Butane, 1,1-dimethoxy

Other names: Butanal dimethyl acetal
Inchi: InChI=1S/C6H14O2/c1-4-5-6(7-2)8-3/h6H,4-5H2,1-3H3
InchiKey: DZKUKLGGGNLHNY-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: CCCC(OC)OC
Mol. weight [g/mol]: 118.17
CAS: 4461-87-4

Physical Properties

Property code	Value	Unit	Source
gf	-212.80	kJ/mol	Joback Method
hf	-426.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-467.40 ± 0.80	kJ/mol	NIST Webbook
hfus	10.15	kJ/mol	Joback Method
hvap	41.70	kJ/mol	NIST Webbook
hvap	41.40	kJ/mol	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.405		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	770.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	768.00		NIST Webbook
ripol	969.00		NIST Webbook
ripol	969.00		NIST Webbook
tb	387.00 ± 4.00	K	NIST Webbook
tc	550.20	K	Joback Method
tf	186.84	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.59	J/mol×K	381.08	Joback Method
cpg	214.84	J/mol×K	409.27	Joback Method
cpg	224.86	J/mol×K	437.45	Joback Method
cpg	234.65	J/mol×K	465.64	Joback Method
cpg	244.19	J/mol×K	493.83	Joback Method
cpg	253.48	J/mol×K	522.01	Joback Method
cpg	262.51	J/mol×K	550.20	Joback Method
dvisc	0.0046299	Pa×s	186.84	Joback Method
dvisc	0.0018547	Pa×s	219.21	Joback Method
dvisc	0.0009402	Pa×s	251.59	Joback Method
dvisc	0.0005565	Pa×s	283.96	Joback Method
dvisc	0.0003667	Pa×s	316.33	Joback Method
dvisc	0.0002611	Pa×s	348.71	Joback Method
dvisc	0.0001969	Pa×s	381.08	Joback Method
hvapt	41.20	kJ/mol	316.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4461874&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/14-540-6/Butane-1-1-dimethoxy.pdf
Generated by Cheméo on 2025-12-19 14:17:50.884110241 +0000 UTC m=+5902068.414150905.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.