

Butane, 1-(2-methoxyethoxy)-

Other names:	1-(2-Methoxyethoxy)butane 1-Butoxy-2-methoxyethane Ethane, 1-butoxy-2-methoxy- butyl 2-methoxyethyl ether
Inchi:	InChI=1S/C7H16O2/c1-3-4-5-9-7-6-8-2/h3-7H2,1-2H3
InchiKey:	XDFQEFFFBRPGSMC-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCCCOCCOC
Mol. weight [g/mol]:	132.20
CAS:	13343-98-1

Physical Properties

Property code	Value	Unit	Source
gf	-201.94	kJ/mol	Joback Method
hf	-452.25	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	47.84	kJ/mol	NIST Webbook
hvap	47.83 ± 0.05	kJ/mol	NIST Webbook
hvap	47.80 ± 0.10	kJ/mol	NIST Webbook
log10ws	-0.93		Crippen Method
logp	1.450		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	420.45 ± 0.30	K	NIST Webbook
tb	420.00 ± 4.00	K	NIST Webbook
tb	419.70	K	NIST Webbook
tc	569.26	K	Joback Method
tf	213.11	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.65	J/mol×K	569.26	Joback Method

cpg	295.82	J/mol×K	541.78	Joback Method
cpg	285.69	J/mol×K	514.30	Joback Method
cpg	275.28	J/mol×K	486.83	Joback Method
cpg	264.58	J/mol×K	459.35	Joback Method
cpg	253.59	J/mol×K	431.88	Joback Method
cpg	242.33	J/mol×K	404.40	Joback Method
dvisc	0.0029460	Pa×s	213.11	Joback Method
dvisc	0.0001992	Pa×s	404.40	Joback Method
dvisc	0.0002575	Pa×s	372.52	Joback Method
dvisc	0.0003493	Pa×s	340.64	Joback Method
dvisc	0.0005047	Pa×s	308.75	Joback Method
dvisc	0.0007936	Pa×s	276.87	Joback Method
dvisc	0.0014040	Pa×s	244.99	Joback Method
hvapt	38.48	kJ/mol	419.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63500e+01
Coeff. B	-4.24415e+03
Coeff. C	-5.79310e+01
Temperature range (K), min.	322.16
Temperature range (K), max.	442.42

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13343981&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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

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
hvac:	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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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