

Butane, 1-propoxy-

Other names:	Butyl propyl ether Ether, butyl propyl
Inchi:	InChI=1S/C7H16O/c1-3-5-7-8-6-4-2/h3-7H2,1-2H3
InchiKey:	YGZQJYIITOMTMD-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCOCCC
Mol. weight [g/mol]:	116.20
CAS:	3073-92-5

Physical Properties

Property code	Value	Unit	Source
gf	-96.94	kJ/mol	Joback Method
hf	-320.03	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	40.26	kJ/mol	NIST Webbook
log10ws	-1.84		Crippen Method
logp	2.213		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	780.00		NIST Webbook
rinpol	780.00		NIST Webbook
ripol	870.00		NIST Webbook
tb	390.30	K	NIST Webbook
tb	389.90 ± 1.00	K	NIST Webbook
tb	391.20	K	NIST Webbook
tc	546.34	K	Joback Method
tf	190.88	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.44	J/mol×K	381.98	Joback Method
cpg	229.92	J/mol×K	409.37	Joback Method

cpg	241.06	J/mol×K	436.77	Joback Method
cpg	251.87	J/mol×K	464.16	Joback Method
cpg	262.35	J/mol×K	491.56	Joback Method
cpg	272.49	J/mol×K	518.95	Joback Method
cpg	282.30	J/mol×K	546.34	Joback Method
dvisc	0.0039006	Pa×s	190.88	Joback Method
dvisc	0.0017217	Pa×s	222.73	Joback Method
dvisc	0.0009325	Pa×s	254.58	Joback Method
dvisc	0.0005789	Pa×s	286.43	Joback Method
dvisc	0.0003953	Pa×s	318.28	Joback Method
dvisc	0.0002894	Pa×s	350.13	Joback Method
dvisc	0.0002231	Pa×s	381.98	Joback Method
hvapt	33.72	kJ/mol	391.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3073925&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1016.mol

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
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

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