

Butyl hexyl ether

Other names:	1-butoxyhexane
Inchi:	InChI=1S/C10H22O/c1-3-5-7-8-10-11-9-6-4-2/h3-10H2,1-2H3
InchiKey:	QCYFOZWGKXDJJA-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCOCCCC
Mol. weight [g/mol]:	158.28
CAS:	54459-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-71.68	kJ/mol	Joback Method
hf	-381.95	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	53.20 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.10		Crippen Method
logp	3.383		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
tb	450.62	K	Joback Method
tc	613.22	K	Joback Method
tf	224.69	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.40	J/molxK	450.62	Joback Method
cpg	411.42	J/molxK	586.12	Joback Method
cpg	398.57	J/molxK	559.02	Joback Method
cpg	385.25	J/molxK	531.92	Joback Method
cpg	371.45	J/molxK	504.82	Joback Method
cpg	357.17	J/molxK	477.72	Joback Method

cpg	423.80	J/mol×K	613.22	Joback Method
dvisc	0.0002026	Paxs	450.62	Joback Method
dvisc	0.0002676	Paxs	412.97	Joback Method
dvisc	0.0003736	Paxs	375.31	Joback Method
dvisc	0.0005620	Paxs	337.65	Joback Method
dvisc	0.0009367	Paxs	300.00	Joback Method
dvisc	0.0018076	Paxs	262.35	Joback Method
dvisc	0.0043485	Paxs	224.69	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=C54459711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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