

1-Butoxy-2-ethylhexane

Other names:	Ether, butyl 2-ethylhexyl
Inchi:	InChI=1S/C12H26O/c1-4-7-9-12(6-3)11-13-10-8-5-2/h12H,4-11H2,1-3H3
InchiKey:	XIUZCZSOJYCCTG-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCOCC(CC)CCCC
Mol. weight [g/mol]:	186.33
CAS:	62625-25-6

Physical Properties

Property code	Value	Unit	Source
gf	-57.28	kJ/mol	Joback Method
hf	-428.51	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	4.019		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
tb	495.94	K	Joback Method
tc	660.05	K	Joback Method
tf	232.23	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.78	J/mol×K	495.94	Joback Method
cpg	452.60	J/mol×K	523.29	Joback Method
cpg	468.81	J/mol×K	550.64	Joback Method
cpg	484.43	J/mol×K	577.99	Joback Method
cpg	499.48	J/mol×K	605.34	Joback Method
cpg	513.95	J/mol×K	632.69	Joback Method
cpg	527.85	J/mol×K	660.05	Joback Method
dvisc	0.0065287	Pa×s	232.23	Joback Method

dvisc	0.0021806	Pa×s	276.18	Joback Method
dvisc	0.0009842	Pa×s	320.13	Joback Method
dvisc	0.0005383	Pa×s	364.09	Joback Method
dvisc	0.0003353	Pa×s	408.04	Joback Method
dvisc	0.0002290	Pa×s	451.99	Joback Method
dvisc	0.0001673	Pa×s	495.94	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=C62625256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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