

butyl dodecyl ether

Inchi:	InChI=1S/C16H34O/c1-3-5-7-8-9-10-11-12-13-14-16-17-15-6-4-2/h3-16H2,1-2H3
InchiKey:	NMMIRFKUKVHGTQ-UHFFFAOYSA-N
Formula:	C16H34O
SMILES:	CCCCCCCCCCCCOCCCC
Mol. weight [g/mol]:	242.44
CAS:	7289-38-5

Physical Properties

Property code	Value	Unit	Source
af	0.7782		Cheméo Relay (1.0)
gf	-21.16	kJ/mol	Joback Method
hf	-503.84	kJ/mol	Cheméo Relay (1.0)
hfus	38.38	kJ/mol	Joback Method
hvap	79.76	kJ/mol	Cheméo Relay (1.0)
ie	9.42	eV	Cheméo Relay (1.0)
log10ws	-6.26		Cheméo Relay (1.0)
logp	5.724		Crippen Method
mcvol	242.170	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
tb	550.23	K	Cheméo Relay (1.0)
tc	723.40	K	Cheméo Relay (1.0)
tf	254.43	K	Cheméo Relay (1.0)
vc	0.960	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.59	J/mol×K	587.90	Joback Method
cpg	662.46	J/mol×K	614.43	Joback Method
cpg	680.61	J/mol×K	640.97	Joback Method
cpg	698.07	J/mol×K	667.50	Joback Method
cpg	714.84	J/mol×K	694.03	Joback Method
cpg	730.94	J/mol×K	720.56	Joback Method
cpg	746.38	J/mol×K	747.10	Joback Method

dvisc	0.0033879	Pa×s	292.31	Joback Method
dvisc	0.0013014	Pa×s	341.57	Joback Method
dvisc	0.0006363	Pa×s	390.84	Joback Method
dvisc	0.0003651	Pa×s	440.11	Joback Method
dvisc	0.0002343	Pa×s	489.37	Joback Method
dvisc	0.0001631	Pa×s	538.63	Joback Method
dvisc	0.0001206	Pa×s	587.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7289385&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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