

BENZENE, (BUTOXYMETHYL)-

Other names:	Ether, benzyl butyl Benzyl butyl ether Benzyl n-butyl ether n-Butyl benzyl ether Ether, benzyl n-butyl
Inchi:	InChI=1S/C11H16O/c1-2-3-9-12-10-11-7-5-4-6-8-11/h4-8H,2-3,9-10H2,1H3
InchiKey:	MAYUYFCAPVDYBQ-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CCCCOCc1ccccc1
Mol. weight [g/mol]:	164.25

Physical Properties

Property code	Value	Unit	Source
af	0.4954		Cheméo Relay (1.0)
gf	49.15	kJ/mol	Joback Method
hf	-149.99	kJ/mol	Cheméo Relay (1.0)
hfus	19.47	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Cheméo Relay (1.0)
ie	8.75	eV	Cheméo Relay (1.0)
log10ws	-2.60		Cheméo Relay (1.0)
logp	3.003		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1238.00		NIST Webbook
ripol	1613.00		NIST Webbook
tb	477.31	K	Cheméo Relay (1.0)
tc	697.15	K	Cheméo Relay (1.0)
tf	205.95	K	Cheméo Relay (1.0)
vc	0.546	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.53	J/mol×K	500.18	Joback Method

cpg	407.94	J/mol×K	700.57	Joback Method
cpg	396.02	J/mol×K	667.17	Joback Method
cpg	383.41	J/mol×K	633.78	Joback Method
cpg	370.07	J/mol×K	600.38	Joback Method
cpg	355.99	J/mol×K	566.98	Joback Method
cpg	341.15	J/mol×K	533.58	Joback Method
dvisc	0.0004708	Pa×s	381.28	Joback Method
dvisc	0.0001846	Pa×s	500.18	Joback Method
dvisc	0.0002390	Pa×s	460.55	Joback Method
dvisc	0.0003249	Pa×s	420.91	Joback Method
dvisc	0.0028054	Pa×s	262.38	Joback Method
dvisc	0.0007435	Pa×s	341.65	Joback Method
dvisc	0.0013237	Pa×s	302.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.00	K	1.30	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C588670&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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