Alpha-phenylethyl n-butyl ether

Other names: (1-Butoxyethyl)benzene
Inchi: InChI=1S/C12H18O/c1-3-4-10-13-11(2)12-8-6-5-7-9-12/h5-9,11H,3-4,10H2,1-2H3
InchiKey: AQGPVCBVZAHVBN-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CCCCOC(C)c1ccccc1
Mol. weight [g/mol]: 178.27
CAS: 4157-77-1

Physical Properties

Property code	Value	Unit	Source
gf	55.13	kJ/mol	Joback Method
hf	-191.98	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	59.80 ± 0.30	kJ/mol	NIST Webbook
log10ws	-3.49		Crippen Method
logp	3.564		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
tb	522.62	K	Joback Method
tc	724.59	K	Joback Method
tf	258.65	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.16	J/mol×K	522.62	Joback Method
cpg	389.01	J/mol×K	556.28	Joback Method
cpg	404.99	J/mol×K	589.94	Joback Method
cpg	420.13	J/mol×K	623.60	Joback Method
cpg	434.45	J/mol×K	657.27	Joback Method
cpg	447.97	J/mol×K	690.93	Joback Method
cpg	460.72	J/mol×K	724.59	Joback Method
dvisc	0.0039484	Pa×s	258.65	Joback Method

dvisc	0.0015764	Pa×s	302.64	Joback Method
dvisc	0.0007945	Pa×s	346.64	Joback Method
dvisc	0.0004673	Pa×s	390.63	Joback Method
dvisc	0.0003060	Pa×s	434.63	Joback Method
dvisc	0.0002166	Pa×s	478.62	Joback Method
dvisc	0.0001625	Pa×s	522.62	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=C4157771&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