

(3-Methoxyphenyl) methanol, n-butyl ether

Inchi:	InChI=1S/C12H18O2/c1-3-4-8-14-10-11-6-5-7-12(9-11)13-2/h5-7,9H,3-4,8,10H2,1-2H3
InchiKey:	LMLPYBKTRWBXFS-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CCCCOCc1cccc(OC)c1
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-57.06	kJ/mol	Joback Method
hf	-330.39	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	50.06	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.012		Crippen Method
mvol	167.920	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1499.00		NIST Webbook
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tb	550.46	K	Joback Method
tc	747.58	K	Joback Method
tf	308.40	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.56	J/molxK	550.46	Joback Method
cpg	414.33	J/molxK	583.31	Joback Method
cpg	429.38	J/molxK	616.17	Joback Method
cpg	443.72	J/molxK	649.02	Joback Method
cpg	457.36	J/molxK	681.87	Joback Method
cpg	470.30	J/molxK	714.73	Joback Method
cpg	482.54	J/molxK	747.58	Joback Method
dvisc	0.0014761	Paxs	308.40	Joback Method

dvisc	0.0007899	Paxs	348.74	Joback Method
dvisc	0.0004813	Paxs	389.09	Joback Method
dvisc	0.0003218	Paxs	429.43	Joback Method
dvisc	0.0002306	Paxs	469.77	Joback Method
dvisc	0.0001742	Paxs	510.12	Joback Method
dvisc	0.0001371	Paxs	550.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U374438&Units=SI

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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