

3-Phenoxybenzyl alcohol, methyl ether

Other names:	m-Phenoxybenzyl methyl ether
Inchi:	InChI=1S/C14H14O2/c1-15-11-12-6-5-9-14(10-12)16-13-7-3-2-4-8-13/h2-10H,11H2,1H3
InchiKey:	SKSSDFHBOHEHQQ-UHFFFAOYSA-N
Formula:	C14H14O2
SMILES:	<chem>COCc1cccc(Oc2ccccc2)c1</chem>
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
gf	72.19	kJ/mol	Joback Method
hf	-135.14	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	56.79	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.625		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
tb	622.90	K	Joback Method
tc	856.47	K	Joback Method
tf	357.36	K	Joback Method
vc	0.639	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.44	J/mol×K	622.90	Joback Method
cpg	439.89	J/mol×K	661.83	Joback Method
cpg	455.22	J/mol×K	700.76	Joback Method
cpg	469.45	J/mol×K	739.69	Joback Method
cpg	482.63	J/mol×K	778.61	Joback Method
cpg	494.76	J/mol×K	817.54	Joback Method
cpg	505.87	J/mol×K	856.47	Joback Method

dvisc	0.0010891	Paxs	357.36	Joback Method
dvisc	0.0006084	Paxs	401.62	Joback Method
dvisc	0.0003815	Paxs	445.87	Joback Method
dvisc	0.0002603	Paxs	490.13	Joback Method
dvisc	0.0001892	Paxs	534.39	Joback Method
dvisc	0.0001444	Paxs	578.64	Joback Method
dvisc	0.0001145	Paxs	622.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U395174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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