

Benzene, 1-methyl-3-phenoxy-

Other names:	Ether, phenyl m-tolyl m-Methylphenyl phenyl ether m-Phenoxytoluene Phenyl m-tolyl ether 1-Methyl-3-phenoxybenzene 3-Methylphenyl phenyl ether 3-Phenoxytoluene 3-Methyldiphenyl ether Phenyl 3-tolyl ether
Inchi:	InChI=1S/C13H12O/c1-11-6-5-9-13(10-11)14-12-7-3-2-4-8-12/h2-10H,1H3
InchiKey:	UDONPJKEOAWFGI-UHFFFAOYSA-N
Formula:	C13H12O
SMILES:	<chem>Cc1cccc(Oc2ccccc2)c1</chem>
Mol. weight [g/mol]:	184.23
CAS:	3586-14-9

Physical Properties

Property code	Value	Unit	Source
gf	168.77	kJ/mol	Joback Method
hf	17.72	kJ/mol	Joback Method
hfus	18.31	kJ/mol	Joback Method
hvap	52.16	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.787		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	259.00		NIST Webbook
rinpol	259.00		NIST Webbook
tb	545.00 ± 1.00	K	NIST Webbook
tb	545.20	K	NIST Webbook
tc	819.70	K	Joback Method
tf	323.86	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.29	J/molxK	577.60	Joback Method
cpg	365.54	J/molxK	617.95	Joback Method
cpg	380.63	J/molxK	658.30	Joback Method
cpg	394.61	J/molxK	698.65	Joback Method
cpg	407.52	J/molxK	739.00	Joback Method
cpg	419.42	J/molxK	779.35	Joback Method
cpg	430.34	J/molxK	819.70	Joback Method
dvisc	0.0014893	Paxs	323.86	Joback Method
dvisc	0.0008203	Paxs	366.15	Joback Method
dvisc	0.0005112	Paxs	408.44	Joback Method
dvisc	0.0003482	Paxs	450.73	Joback Method
dvisc	0.0002533	Paxs	493.02	Joback Method
dvisc	0.0001937	Paxs	535.31	Joback Method
dvisc	0.0001541	Paxs	577.60	Joback Method

Sources

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=C3586149&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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