

Benzoic acid, 2-phenoxy-, methyl ester

Other names:	Benzoic acid, o-phenoxy-, methyl ester Methyl o-phenoxybenzoate Methyl 2-phenoxybenzoate
Inchi:	InChI=1S/C14H12O3/c1-16-14(15)12-9-5-6-10-13(12)17-11-7-3-2-4-8-11/h2-10H,1H3
InchiKey:	PUGYLBSXMKBSRP-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	COC(=O)c1ccccc1Oc1ccccc1
Mol. weight [g/mol]:	228.24
CAS:	21905-56-6

Physical Properties

Property code	Value	Unit	Source
gf	-56.73	kJ/mol	Joback Method
hf	-247.72	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	63.54	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.265		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	676.77	K	Joback Method
tc	916.60	K	Joback Method
tf	407.29	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.07	J/molxK	676.77	Joback Method
cpg	454.76	J/molxK	716.74	Joback Method
cpg	468.31	J/molxK	756.71	Joback Method
cpg	480.73	J/molxK	796.68	Joback Method

cpg	492.07	J/molxK	836.66	Joback Method
cpg	502.33	J/molxK	876.63	Joback Method
cpg	511.55	J/molxK	916.60	Joback Method
dvisc	0.0009553	Paxs	407.29	Joback Method
dvisc	0.0005676	Paxs	452.20	Joback Method
dvisc	0.0003705	Paxs	497.12	Joback Method
dvisc	0.0002596	Paxs	542.03	Joback Method
dvisc	0.0001921	Paxs	586.94	Joback Method
dvisc	0.0001483	Paxs	631.86	Joback Method
dvisc	0.0001185	Paxs	676.77	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=C21905566&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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