Benzoic acid, 4-phenoxy-

Other names:	Benzoic acid, p-phenoxy-
	p-Phenoxybenzoic acid
	Diphenyl ether 4-carboxylic acid
	4-Phenoxybenzoic acid
Inchi:	InChI=1S/C13H10O3/c14-13(15)10-6-8-12(9-7-10)16-11-4-2-1-3-5-11/h1-9H,(H,14,15)
InchiKey:	RYAQFHLUEMJOMF-UHFFFAOYSA-N
Formula:	C13H10O3
SMILES:	O=C(O)c1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	214.22
CAS:	2215-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-96.97	kJ/mol	Joback Method
hf	-247.09	kJ/mol	Joback Method
hfus	23.99	kJ/mol	Joback Method
hvap	75.58	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.177		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	723.65	K	Joback Method
tc	951.31	K	Joback Method
tf	434.61	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.87	J/mol×K	723.65	Joback Method
cpg	425.06	J/mol×K	761.59	Joback Method
cpg	435.34	J/mol×K	799.54	Joback Method
cpg	444.75	J/mol×K	837.48	Joback Method
cpg	453.33	J/mol×K	875.43	Joback Method

cpg	461.11	J/mol×K	913.37	Joback Method
cpg	468.14	J/mol×K	951.31	Joback Method
dvisc	0.0010708	Pa×s	434.61	Joback Method
dvisc	0.0004645	Pa×s	482.78	Joback Method
dvisc	0.0002344	Pa×s	530.96	Joback Method
dvisc	0.0001326	Pa×s	579.13	Joback Method
dvisc	0.0000819	Pa×s	627.30	Joback Method
dvisc	0.0000541	Pa×s	675.48	Joback Method
dvisc	0.0000378	Pa×s	723.65	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2215772&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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