

Benzene, 1-chloro-4-phenoxy-

Other names:	Ether, p-chlorophenyl phenyl p-Chlorodiphenyl oxide p-Chlorophenyl phenyl ether 1-Chloro-4-phenoxybenzene 4-Chlorodiphenyl ether 4-Chlorophenyl phenyl ether
Inchi:	InChI=1S/C12H9ClO/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9H
InchiKey:	PGPNJCAMHOJTEF-UHFFFAOYSA-N
Formula:	C12H9ClO
SMILES:	Clc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	204.65
CAS:	7005-72-3

Physical Properties

Property code	Value	Unit	Source
gf	148.42	kJ/mol	Joback Method
hf	22.62	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	4.132		Crippen Method
mcvol	150.530	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1546.50		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1546.50		NIST Webbook
rinpol	270.90		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	592.15	K	Joback Method
tc	843.25	K	Joback Method
tf	342.51	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.17	J/molxK	592.15	Joback Method
cpg	388.95	J/molxK	801.40	Joback Method
cpg	378.84	J/molxK	759.55	Joback Method
cpg	367.76	J/molxK	717.70	Joback Method
cpg	355.65	J/molxK	675.85	Joback Method
cpg	342.47	J/molxK	634.00	Joback Method
cpg	398.13	J/molxK	843.25	Joback Method
dvisc	0.0001652	Paxs	592.15	Joback Method
dvisc	0.0002065	Paxs	550.54	Joback Method
dvisc	0.0002678	Paxs	508.94	Joback Method
dvisc	0.0003636	Paxs	467.33	Joback Method
dvisc	0.0005242	Paxs	425.72	Joback Method
dvisc	0.0008182	Paxs	384.12	Joback Method
dvisc	0.0014227	Paxs	342.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	434.70	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7005723&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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