

Benzene, 1-phenoxy-4-(2-chloroethoxy)-

Inchi:	InChI=1S/C14H13ClO2/c15-10-11-16-12-6-8-14(9-7-12)17-13-4-2-1-3-5-13/h1-9H,10-11H
InchiKey:	ACDJKCYEQDTWGR-UHFFFAOYSA-N
Formula:	C14H13ClO2
SMILES:	CICCOc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	248.71
CAS:	61435-02-7

Physical Properties

Property code	Value	Unit	Source
gf	60.26	kJ/mol	Joback Method
hf	-150.88	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	4.096		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	660.33	K	Joback Method
tc	896.94	K	Joback Method
tf	387.28	K	Joback Method
vc	0.689	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.34	J/molxK	660.33	Joback Method
cpg	465.57	J/molxK	699.76	Joback Method
cpg	479.67	J/molxK	739.20	Joback Method
cpg	492.68	J/molxK	778.63	Joback Method
cpg	504.63	J/molxK	818.07	Joback Method
cpg	515.53	J/molxK	857.50	Joback Method
cpg	525.44	J/molxK	896.94	Joback Method
dvisc	0.0009749	Paxs	387.28	Joback Method
dvisc	0.0005573	Paxs	432.79	Joback Method

dvisc	0.0003543	Paxs	478.30	Joback Method
dvisc	0.0002437	Paxs	523.80	Joback Method
dvisc	0.0001780	Paxs	569.31	Joback Method
dvisc	0.0001362	Paxs	614.82	Joback Method
dvisc	0.0001081	Paxs	660.33	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=C61435027&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/118-229-7/Benzene-1-phenoxy-4-2-chloroethoxy.pdf>

Generated by Cheméo on 2024-04-25 08:08:08.615788549 +0000 UTC m=+16321737.536365864.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.