1,3-Diphenoxypropane

Other names: Benzene, 1,1'-[1,3-propanediylbis(oxy)]bis-
Inchi: InChI=1S/C15H16O2/c1-3-8-14(9-4-1)16-12-7-13-17-15-10-5-2-6-11-15/h1-6,8-11H,7,12
InchiKey: HZIVULLSUOJNPX-UHFFFAOYSA-N
Formula: C15H16O2
SMILES: c1ccc(OCCCOc2ccccc2)cc1
Mol. weight [g/mol]: 228.29
CAS: 726-44-3

Physical Properties

Property code	Value	Unit	Source
gf	90.24	kJ/mol	Joback Method
hf	-144.31	kJ/mol	Joback Method
hfus	25.06	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
ie	8.46 ± 0.05	eV	NIST Webbook
log10ws	-3.78		Crippen Method
logp	3.535		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	612.20	K	NIST Webbook
tc	868.87	K	Joback Method
tf	356.11	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.74	J/mol×K	640.80	Joback Method
cpg	549.09	J/mol×K	830.86	Joback Method
cpg	536.45	J/mol×K	792.85	Joback Method
cpg	522.74	J/mol×K	754.84	Joback Method
cpg	507.90	J/mol×K	716.82	Joback Method
cpg	491.92	J/mol×K	678.81	Joback Method
cpg	560.68	J/mol×K	868.87	Joback Method

dvisc	0.0001049	Pa×s	640.80	Joback Method
dvisc	0.0001352	Pa×s	593.35	Joback Method
dvisc	0.0001821	Pa×s	545.90	Joback Method
dvisc	0.0002597	Pa×s	498.45	Joback Method
dvisc	0.0003989	Pa×s	451.01	Joback Method
dvisc	0.0006779	Pa×s	403.56	Joback Method
dvisc	0.0013267	Pa×s	356.11	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=C726443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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