1,2-PROPANEDIOL, 3-(4-CHLOROPHENOXY)-

Other names:	1,2-Propanediol, 3-(4-chlorophenoxy)- 1,2-Propanediol, 3-(p-chlorophenoxy)- p-Chlorophenyl glyceryl ether p-Chlorophenyl-«alpha»-glyceryl ether Adermykon Chlorophenesin Demykon Gecophen Glycerol «alpha»-p-chlorophenyl ether Mycil 3-(p-Chlorophenoxy)-1,2-propanediol 3-(p-Chlorophenoxy)propane-1,2-diol 3-(4-Chlorophenoxy)-1,2-propanediol Gechophen NSC 6401
Inchi:	InChI=1S/C9H11ClO3/c10-7-1-3-9(4-2-7)13-6-8(12)5-11/h1-4,8,11-12H,5-6H2
InchiKey:	MXOAEAUPQDYUQM-UHFFFAOYSA-N
Formula:	C9H11ClO3
SMILES:	OCC(O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	202.64

Physical Properties

Property code	Value	Unit	Source
hfus	22.76	kJ/mol	Joback Method
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-1.62		Cheméo Relay (1.0)
logp	1.072		Crippen Method
mcvol	143.760	ml/mol	McGowan Method
tb	607.85	K	Cheméo Relay (1.0)
tf	338.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	359.81	J/mol×K	680.75	Joback Method
cpg	368.68	J/mol×K	712.72	Joback Method
cpg	377.04	J/mol×K	744.69	Joback Method
cpg	384.88	J/mol×K	776.66	Joback Method
cpg	392.24	J/mol×K	808.63	Joback Method
cpg	399.11	J/mol×K	840.59	Joback Method
cpg	405.52	J/mol×K	872.56	Joback Method
dvisc	0.0031082	Pa×s	388.92	Joback Method
dvisc	0.0007638	Pa×s	437.56	Joback Method
dvisc	0.0002486	Pa×s	486.20	Joback Method
dvisc	0.0000992	Pa×s	534.84	Joback Method
dvisc	0.0000461	Pa×s	583.47	Joback Method
dvisc	0.0000241	Pa×s	632.11	Joback Method
dvisc	0.0000139	Pa×s	680.75	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104290&Units=SI

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

hfus: Enthalpy of fusion at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point