Chlorphenesin

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]:	202.63
CAS:	104-29-0

Physical Properties

Property code	Value	Unit	Source
gf	-265.33	kJ/mol	Joback Method
hf	-461.73	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	78.33	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.072		Crippen Method
mcvol	143.760	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	680.75	K	Joback Method
tc	872.56	K	Joback Method
tf	388.92	K	Joback Method
vc	0.530	m3/kmol	Joback Method

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

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=C104290&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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