1,2-Propanediol, 3-phenoxy-

Other names:	Antodyne
	Glycerol «alpha»-monophenyl ether
	Glycerol «alpha»-phenyl ether
	Phenol glyceryl ether
	Phenylglyceryl ether
	3-Phenoxy-1,2-propanediol
	Phenol glycerol ether
	Phenol-glycerinaether
	Phenyl-«alpha»-glycerol ether
	Antodyn
	1-Fenoxy-2,3-propandiol
	1-Phenoxy-2,3-propanediol
	U 27,462
	1,2-Dihydroxy-3-phenoxypropane
	NSC 406489
	«alpha»-Phenyl monoglyceryl ether
	3-phenoxypropane-1,2-diol
Inchi:	InChI=1S/C9H12O3/c10-6-8(11)7-12-9-4-2-1-3-5-9/h1-5,8,10-11H,6-7H2
InchiKey:	FNQIYTUXOKTMDM-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	OCC(O)COc1ccccc1
Mol. weight [g/mol]:	168.19
CAS:	538-43-2

Physical Properties

Property code	Value	Unit	Source
gf	-243.77	kJ/mol	Joback Method
hf	-434.52	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	73.28	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.419		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	588.20	K	NIST Webbook
tc	825.22	K	Joback Method
tf	346.48	K	Joback Method

vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.34	J/mol×K	825.22	Joback Method
cpg	338.80	J/mol×K	638.34	Joback Method
cpg	348.52	J/mol×K	669.49	Joback Method
cpg	357.70	J/mol×K	700.63	Joback Method
cpg	366.35	J/mol×K	731.78	Joback Method
cpg	374.50	J/mol×K	762.92	Joback Method
cpg	382.16	J/mol×K	794.07	Joback Method
dvisc	0.0000188	Pa×s	638.34	Joback Method
dvisc	0.0104619	Pa×s	346.48	Joback Method
dvisc	0.0019072	Pa×s	395.12	Joback Method
dvisc	0.0005049	Pa×s	443.77	Joback Method
dvisc	0.0001738	Pa×s	492.41	Joback Method
dvisc	0.0000725	Pa×s	541.05	Joback Method
dvisc	0.0000349	Pa×s	589.70	Joback Method
hfust	28.00	kJ/mol	331.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C538432&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
hfust:	Enthalpy of fusion at a given temperature
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