3-(2-Cyclohexylphenoxy)-1,2-propanediol

Inchi: InChI=1S/C15H22O3/c16-10-13(17)11-18-15-9-5-4-8-14(15)12-6-2-1-3-7-12/h4-5,8-9,12-
InchiKey: GEGQXICLYBLOQI-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: OCC(O)COc1ccccc1C1CCCCC1
Mol. weight [g/mol]: 250.33
CAS: 132801-79-7

Physical Properties

Property code	Value	Unit	Source
gf	-178.43	kJ/mol	Joback Method
hf	-515.51	kJ/mol	Joback Method
hfus	25.93	kJ/mol	Joback Method
hvap	87.73	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.466		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
tb	800.15	K	Joback Method
tc	1003.59	K	Joback Method
tf	434.00	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.84	J/mol×K	800.15	Joback Method
cpg	657.93	J/mol×K	834.06	Joback Method
cpg	671.02	J/mol×K	867.96	Joback Method
cpg	683.15	J/mol×K	901.87	Joback Method
cpg	694.33	J/mol×K	935.77	Joback Method
cpg	704.62	J/mol×K	969.68	Joback Method
cpg	714.04	J/mol×K	1003.59	Joback Method
dvisc	0.0013530	Pa×s	434.00	Joback Method
dvisc	0.0002895	Pa×s	495.02	Joback Method

dvisc	0.0000869	Pa×s	556.05	Joback Method
dvisc	0.0000331	Pa×s	617.08	Joback Method
dvisc	0.0000150	Pa×s	678.10	Joback Method
dvisc	0.0000077	Pa×s	739.12	Joback Method
dvisc	0.0000044	Pa×s	800.15	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=C132801797&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
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