

1,3-Bis(2-methylphenoxy)-2-propanol

Inchi:	InChI=1S/C17H20O3/c1-13-7-3-5-9-16(13)19-11-15(18)12-20-17-10-6-4-8-14(17)2/h3-10
InchiKey:	GZSFOYFMSYYKJH-UHFFFAOYSA-N
Formula:	C17H20O3
SMILES:	Cc1ccccc1OCC(O)COc1ccccc1C
Mol. weight [g/mol]:	272.34
CAS:	17181-49-6

Physical Properties

Property code	Value	Unit	Source
gf	-51.44	kJ/mol	Joback Method
hf	-366.04	kJ/mol	Joback Method
hfus	30.03	kJ/mol	Joback Method
hvap	80.42	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.122		Crippen Method
mvol	220.480	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
tb	788.26	K	Joback Method
tc	1000.28	K	Joback Method
tf	449.51	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.35	J/molxK	788.26	Joback Method
cpg	653.54	J/molxK	823.60	Joback Method
cpg	666.71	J/molxK	858.93	Joback Method
cpg	678.86	J/molxK	894.27	Joback Method
cpg	690.03	J/molxK	929.60	Joback Method
cpg	700.25	J/molxK	964.94	Joback Method
cpg	709.52	J/molxK	1000.28	Joback Method
dvisc	0.0006017	Paxs	449.51	Joback Method
dvisc	0.0002298	Paxs	505.97	Joback Method

dvisc	0.0001065	Paxs	562.43	Joback Method
dvisc	0.0000568	Paxs	618.88	Joback Method
dvisc	0.0000336	Paxs	675.34	Joback Method
dvisc	0.0000216	Paxs	731.80	Joback Method
dvisc	0.0000148	Paxs	788.26	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=C17181496&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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