

Propane, 2,2-bis[4-(2-hydroxypropyloxy)-phenyl]-

Other names:1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol

Inchi:InChI=1S/C21H28O4/c1-15(22)13-24-19-9-5-17(6-10-19)21(3,4)18-7-11-20(12-8-18)25-1

InchiKey:MIUUNYUUEFHIHM-UHFFFAOYSA-N

Formula:C21H28O4

SMILES:CC(O)COc1ccc(C(C)(C)c2ccc(OCC(C)O)cc2)cc1

Mol. weight [g/mol]:344.44

CAS:116-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-154.18	kJ/mol	Joback Method
hf	-614.86	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	104.32	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.532		Crippen Method
mcvol	282.710	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
tb	968.29	K	Joback Method
tc	1188.30	K	Joback Method
tf	542.83	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.43	J/mol×K	968.29	Joback Method
cpg	978.95	J/mol×K	1151.63	Joback Method
cpg	970.13	J/mol×K	1114.96	Joback Method
cpg	960.43	J/mol×K	1078.30	Joback Method
cpg	949.79	J/mol×K	1041.63	Joback Method
cpg	938.15	J/mol×K	1004.96	Joback Method
cpg	986.97	J/mol×K	1188.30	Joback Method
dvisc	0.0000006	Pa×s	968.29	Joback Method

dvisc	0.0000010	Pa×s	897.38	Joback Method
dvisc	0.0000018	Pa×s	826.47	Joback Method
dvisc	0.0000036	Pa×s	755.56	Joback Method
dvisc	0.0000085	Pa×s	684.65	Joback Method
dvisc	0.0000244	Pa×s	613.74	Joback Method
dvisc	0.0000923	Pa×s	542.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116370&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
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

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