

1,3-Bis([1,1'-biphenyl]-4-yloxy)-2-propanol

Inchi:	InChI=1S/C27H24O3/c28-25(19-29-26-15-11-23(12-16-26)21-7-3-1-4-8-21)20-30-27-17-
InchiKey:	SWSSHWKHGNWTHJ-UHFFFAOYSA-N
Formula:	C27H24O3
SMILES:	OC(COc1ccc(-c2ccccc2)cc1)COc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	396.48
CAS:	22820-60-6

Physical Properties

Property code	Value	Unit	Source
gf	257.58	kJ/mol	Joback Method
hf	-99.38	kJ/mol	Joback Method
hfus	44.01	kJ/mol	Joback Method
hvap	107.23	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	5.839		Crippen Method
mcvol	313.860	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
tb	1070.42	K	Joback Method
tc	1322.81	K	Joback Method
tf	615.05	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.99	J/molxK	1070.42	Joback Method
cpg	1052.94	J/molxK	1280.74	Joback Method
cpg	1046.52	J/molxK	1238.68	Joback Method
cpg	1039.13	J/molxK	1196.61	Joback Method
cpg	1030.66	J/molxK	1154.55	Joback Method
cpg	1020.99	J/molxK	1112.48	Joback Method
cpg	1058.50	J/molxK	1322.81	Joback Method
dvisc	0.0000026	Paxs	1070.42	Joback Method
dvisc	0.0000037	Paxs	994.52	Joback Method

dvisc	0.0000055	Paxs	918.63	Joback Method
dvisc	0.0000089	Paxs	842.73	Joback Method
dvisc	0.0000158	Paxs	766.84	Joback Method
dvisc	0.0000319	Paxs	690.94	Joback Method
dvisc	0.0000764	Paxs	615.05	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=C22820606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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