

4, 4'-Isopropylidenebis (2-isopropylphenol)

Inchi:	InChI=1S/C21H28O2/c1-13(2)17-11-15(7-9-19(17)22)21(5,6)16-8-10-20(23)18(12-16)14
InchiKey:	IJWIRZQYWANBMP-UHFFFAOYSA-N
Formula:	C21H28O2
SMILES:	CC(C)c1cc(C(C)(C)c2ccc(O)c(C(C)C)c2)ccc1O
Mol. weight [g/mol]:	312.45
CAS:	127-54-8

Physical Properties

Property code	Value	Unit	Source
gf	20.22	kJ/mol	Joback Method
hf	-400.58	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	92.17	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.670		Crippen Method
mcvol	270.970	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
tb	900.33	K	Joback Method
tc	1145.40	K	Joback Method
tf	600.17	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.07	J/molxK	900.33	Joback Method
cpg	881.89	J/molxK	941.17	Joback Method
cpg	899.36	J/molxK	982.02	Joback Method
cpg	916.69	J/molxK	1022.86	Joback Method
cpg	934.14	J/molxK	1063.71	Joback Method
cpg	951.93	J/molxK	1104.55	Joback Method
cpg	970.30	J/molxK	1145.40	Joback Method
dvisc	0.0000075	Paxs	600.17	Joback Method
dvisc	0.0000028	Paxs	650.20	Joback Method

dvisc	0.0000012	Paxs	700.22	Joback Method
dvisc	0.0000006	Paxs	750.25	Joback Method
dvisc	0.0000003	Paxs	800.28	Joback Method
dvisc	0.0000002	Paxs	850.30	Joback Method
dvisc	0.0000001	Paxs	900.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C127548&Units=SI

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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