

O-(BIS(P-HYDROXYPHENYL)METHYL)BENZYL ALCOHOL

Other names:

- o-(Bis(p-hydroxyphenyl)methyl)benzyl alcohol
- Benzyl alcohol, o-(bis(p-hydroxyphenyl)methyl)-
- Bis-(4-hydroxyphenyl)-(2-hydroxymethylphenyl)methane
- Egmol
- Normolax
- Phenolphthalol
- Regmolax
- Velaxin
- 2-[Bis(4-hydroxyphenyl)methyl]benzenemethanol
- Regolax
- NSC 91527

Inchi: InChI=1S/C20H18O3/c21-13-16-3-1-2-4-19(16)20(14-5-9-17(22)10-6-14)15-7-11-18(23)1

InchiKey: CREICILGVGNQBH-UHFFFAOYSA-N

Formula: C20H18O3

SMILES: OCc1ccccc1C(c1ccc(O)cc1)c1ccc(O)cc1

Mol. weight [g/mol]: 306.36

Physical Properties

Property code	Value	Unit	Source
hfus	41.42	kJ/mol	Joback Method
ie	8.17	eV	Cheméo Relay (1.0)
log10ws	-3.96		Cheméo Relay (1.0)
logp	3.770		Crippen Method
mcvol	238.990	ml/mol	McGowan Method
tf	449.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.86	J/mol×K	995.00	Joback Method
cpg	769.47	J/mol×K	1037.25	Joback Method
cpg	784.38	J/mol×K	1079.50	Joback Method
cpg	799.86	J/mol×K	1121.75	Joback Method
cpg	816.14	J/mol×K	1164.00	Joback Method

cpg	833.49	J/mol×K	1206.25	Joback Method
cpg	852.15	J/mol×K	1248.50	Joback Method
dvisc	0.0000010	Pa×s	676.20	Joback Method
dvisc	0.0000004	Pa×s	729.33	Joback Method
dvisc	0.0000002	Pa×s	782.47	Joback Method
dvisc	8.1319212e-08	Pa×s	835.60	Joback Method
dvisc	4.2632568e-08	Pa×s	888.73	Joback Method
dvisc	2.4039860e-08	Pa×s	941.87	Joback Method
dvisc	1.4411043e-08	Pa×s	995.00	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81925&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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