3,5-di-t-Butyl-4-hydroxybenzyl ether

Other names:	3,5-di-tert-Butyl-4-hydroxybenzyl ether Phenol, 4,4'-[oxybis(methylene)]bis[2,6-bis(1,1-dimethylethyl)- 4,4'-[Oxybis(methylene)bis[2,6-bis(1,1-dimethylethyl)phenol]
Inchi:	InChI=1S/C30H46O3/c1-27(2,3)21-13-19(14-22(25(21)31)28(4,5)6)17-33-18-20-15-23(29
InchiKey:	HWCZIOQRLAPHDF-UHFFFAOYSA-N
Formula:	C30H46O3
SMILES:	CC(C)(C)c1cc(COCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O
Mol. weight [g/mol]:	454.68
CAS:	6922-60-7

Physical Properties

Property code	Value	Unit	Source
gf	-14.86	kJ/mol	Joback Method
hf	-757.19	kJ/mol	Joback Method
hfus	43.08	kJ/mol	Joback Method
hvap	112.83	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	8.005		Crippen Method
mcvol	403.650	ml/mol	McGowan Method
pc	1014.89	kPa	Joback Method
tb	1129.82	K	Joback Method
tc	1385.50	K	Joback Method
tf	786.13	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1466.68	J/mol×K	1129.82	Joback Method
cpg	1617.37	J/mol×K	1342.89	Joback Method
cpg	1583.51	J/mol×K	1300.27	Joback Method
cpg	1551.88	J/mol×K	1257.66	Joback Method
cpg	1522.11	J/mol×K	1215.05	Joback Method
cpg	1493.84	J/mol×K	1172.43	Joback Method

cpg	1653.83	J/mol×K	1385.50	Joback Method
dvisc	3.9643264e-09	Pa×s	1129.82	Joback Method
dvisc	6.0971695e-09	Pa×s	1072.54	Joback Method
dvisc	9.8442786e-09	Pa×s	1015.26	Joback Method
dvisc	1.6831418e-08	Pa×s	957.97	Joback Method
dvisc	3.0809582e-08	Pa×s	900.69	Joback Method
dvisc	6.1223195e-08	Pa×s	843.41	Joback Method
dvisc	0.0000001	Pa×s	786.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6922607&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