

Phenol, 4,4'-butylidene bis(2,6-di-tert-butyl)-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C32H50O2/c1-14-15-22(20-16-23(29(2,3)4)27(33)24(17-20)30(5,6)7)21-18-25

FLSKKFALEYBSJE-UHFFFAOYSA-N

C32H50O2

CCCC(c1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1)c1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1

466.74

19072-79-8

Physical Properties

Property code	Value	Unit	Source
gf	104.54	kJ/mol	Joback Method
hf	-671.53	kJ/mol	Joback Method
hfus	43.55	kJ/mol	Joback Method
hvap	114.48	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	9.220		Crippen Method
mcvol	425.960	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
tb	1152.72	K	Joback Method
tc	1412.17	K	Joback Method
tf	771.44	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1574.16	J/mol×K	1152.72	Joback Method
cpg	1747.49	J/mol×K	1368.93	Joback Method
cpg	1707.97	J/mol×K	1325.68	Joback Method
cpg	1671.30	J/mol×K	1282.44	Joback Method
cpg	1637.06	J/mol×K	1239.20	Joback Method
cpg	1604.82	J/mol×K	1195.96	Joback Method
cpg	1790.29	J/mol×K	1412.17	Joback Method
dvisc	3.2793277e-09	Pa×s	1152.72	Joback Method
dvisc	5.2270146e-09	Pa×s	1089.17	Joback Method

dvisc	8.8269792e-09	Pa×s	1025.63	Joback Method
dvisc	1.5974658e-08	Pa×s	962.08	Joback Method
dvisc	3.1440546e-08	Pa×s	898.53	Joback Method
dvisc	6.8597338e-08	Pa×s	834.99	Joback Method
dvisc	0.0000002	Pa×s	771.44	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=C19072798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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