2,2'-Ethylidenebis(4,6-di-tert-butylphenol)

Other names: Phenol, 2,2'-ethylidenebis[4,6-bis(1,1-dimethylethyl)-
2,2'-Ethylidene bis(4,6-di-t-butylphenol)
2,2'-Ethylidenebis (4,5-di-tert.-butylphenol)
Ethylidenebisdibutylphenol
Isonox 129
Vanox 1290

Inchi: InChI=1S/C30H46O2/c1-18(21-14-19(27(2,3)4)16-23(25(21)31)29(8,9)10)22-15-20(28(5,

InchiKey: DXCHWXWXYPEZKM-UHFFFAOYSA-N

Formula: C30H46O2

SMILES: CC(c1cc(C(C)(C)C)cc(C(C)(C)C)c1O)c1cc(C(C)(C)C)cc(C(C)(C)C)c1O

Mol. weight [g/mol]: 438.69

CAS: 35958-30-6

Physical Properties

Property code	Value	Unit	Source
gf	87.70	kJ/mol	Joback Method
hf	-630.25	kJ/mol	Joback Method
hfus	38.37	kJ/mol	Joback Method
hvap	110.03	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	8.440		Crippen Method
mcvol	397.780	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
tb	1106.96	K	Joback Method
tc	1361.39	K	Joback Method
tf	748.90	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1435.50	J/mol×K	1106.96	Joback Method
cpg	1462.87	J/mol×K	1149.37	Joback Method
cpg	1491.41	J/mol×K	1191.77	Joback Method

cpg	1521.52	J/mol×K	1234.18	Joback Method
cpg	1553.58	J/mol×K	1276.58	Joback Method
cpg	1587.99	J/mol×K	1318.99	Joback Method
cpg	1625.13	J/mol×K	1361.39	Joback Method
dvisc	0.0000003	Pa×s	748.90	Joback Method
dvisc	0.0000001	Pa×s	808.58	Joback Method
dvisc	5.0638748e-08	Pa×s	868.25	Joback Method
dvisc	2.5956284e-08	Pa×s	927.93	Joback Method
dvisc	1.4423742e-08	Pa×s	987.61	Joback Method
dvisc	8.5702426e-09	Pa×s	1047.28	Joback Method
dvisc	5.3862306e-09	Pa×s	1106.96	Joback Method

Sources

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=C35958306&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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