

Thymol blue

Other names:	Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[5-methyl-2-(1-methylethyl)-, S,S-dioxide, Thymol, 6,6'-(3H-2,1-benzoxathiol-3-ylidene)di-, S,S-dioxide Thymolsulfonephthalein Thymolsulfophthalein Thymolsulphonphthalein Thymosulfonphthalein Thymolsulfonephalein
Inchi:	InChI=1S/C27H30O5S/c1-15(2)19-13-22(17(5)11-24(19)28)27(21-9-7-8-10-26(21)33(30,
InchiKey:	PRZSXZWFJHEZBJ-UHFFFAOYSA-N
Formula:	C27H30O5S
SMILES:	Cc1cc(O)c(C(C)C)cc1C1(c2cc(C(C)C)c(O)cc2C)OS(=O)(=O)c2ccccc21
Mol. weight [g/mol]:	466.59
CAS:	76-61-9

Physical Properties

Property code	Value	Unit	Source
gf	-341.24	kJ/mol	Joback Method
hf	-807.47	kJ/mol	Joback Method
hfus	61.10	kJ/mol	Joback Method
hvap	131.99	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	5.972		Crippen Method
mcvol	354.850	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
tb	1143.22	K	Joback Method
tc	1406.68	K	Joback Method
tf	885.37	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.89	J/mol×K	1143.22	Joback Method
cpg	1289.84	J/mol×K	1187.13	Joback Method

cpg	1325.53	J/mol×K	1231.04	Joback Method
cpg	1364.42	J/mol×K	1274.95	Joback Method
cpg	1406.96	J/mol×K	1318.86	Joback Method
cpg	1453.60	J/mol×K	1362.77	Joback Method
cpg	1504.79	J/mol×K	1406.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76619&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
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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