

M-cresol, 4,4'-ethylidene bis(6-tert-octyl)-

Inchi: InChI=1S/C32H50O2/c1-22-18-29(33)25(14-10-12-16-31(4,5)6)20-27(22)24(3)28-21-26(3)
InchiKey: IJPNLJSXFNBME-UHFFFAOYSA-N
Formula: C32H50O2
SMILES: Cc1cc(O)c(CCCCC(C)(C)C)cc1C(C)c1cc(CCCCC(C)(C)C)c(O)cc1C
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	98.86	kJ/mol	Joback Method
hf	-654.03	kJ/mol	Joback Method
hfus	58.38	kJ/mol	Joback Method
hvap	117.07	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.384		Crippen Method
mcvol	425.960	ml/mol	McGowan Method
pc	894.27	kPa	Joback Method
tb	1159.18	K	Joback Method
tc	1419.90	K	Joback Method
tf	766.60	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1573.57	J/molxK	1159.18	Joback Method
cpg	1602.78	J/molxK	1202.63	Joback Method
cpg	1632.98	J/molxK	1246.09	Joback Method
cpg	1664.54	J/molxK	1289.54	Joback Method
cpg	1697.83	J/molxK	1332.99	Joback Method
cpg	1733.19	J/molxK	1376.45	Joback Method
cpg	1770.99	J/molxK	1419.90	Joback Method
dvisc	0.0000003	Paxs	766.60	Joback Method
dvisc	0.0000001	Paxs	832.03	Joback Method
dvisc	5.4180014e-08	Paxs	897.46	Joback Method

dvisc	2.7975493e-08	Paxs	962.89	Joback Method
dvisc	1.5712551e-08	Paxs	1028.32	Joback Method
dvisc	9.4556206e-09	Paxs	1093.75	Joback Method
dvisc	6.0260406e-09	Paxs	1159.18	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=B6000797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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