

M-cresol, 4,4'-methylene bis(6-(1,1,3,3-tetramethylbutyl))-

Inchi:	InChI=1S/C31H48O2/c1-20-13-26(32)24(30(9,10)18-28(3,4)5)16-22(20)15-23-17-25(27(
InchiKey:	CAHSZBPNBIEERN-UHFFFAOYSA-N
Formula:	C31H48O2
SMILES:	Cc1cc(O)c(C(C)(C)CC(C)(C)C)cc1Cc1cc(C(C)(C)CC(C)(C)C)c(O)cc1C
Mol. weight [g/mol]:	452.71
CAS:	26292-73-9

Physical Properties

Property code	Value	Unit	Source
gf	98.56	kJ/mol	Joback Method
hf	-645.61	kJ/mol	Joback Method
hfus	44.48	kJ/mol	Joback Method
hvap	112.64	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	8.733		Crippen Method
mcvol	411.870	ml/mol	McGowan Method
pc	965.67	kPa	Joback Method
tb	1130.28	K	Joback Method
tc	1385.81	K	Joback Method
tf	775.17	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1504.38	J/molxK	1130.28	Joback Method
cpg	1533.34	J/molxK	1172.87	Joback Method
cpg	1563.68	J/molxK	1215.46	Joback Method
cpg	1595.80	J/molxK	1258.05	Joback Method
cpg	1630.09	J/molxK	1300.63	Joback Method
cpg	1666.96	J/molxK	1343.22	Joback Method
cpg	1706.80	J/molxK	1385.81	Joback Method
dvisc	0.0000002	Paxs	775.17	Joback Method
dvisc	7.9910699e-08	Paxs	834.36	Joback Method

dvisc	3.8867789e-08	Paxs	893.54	Joback Method
dvisc	2.0675921e-08	Paxs	952.73	Joback Method
dvisc	1.1841485e-08	Paxs	1011.91	Joback Method
dvisc	7.2127040e-09	Paxs	1071.10	Joback Method
dvisc	4.6274152e-09	Paxs	1130.28	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=C26292739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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