

M-cresol, 4,4'-butylidene bis(6-(1-methylcyclohexyl))-

Inchi:	InChI=1S/C32H46O2/c1-6-13-24(25-20-27(29(33)18-22(25)2)31(4)14-9-7-10-15-31)26-2
InchiKey:	NMKVEOZMNCIUQW-UHFFFAOYSA-N
Formula:	C32H46O2
SMILES:	CCCC(c1cc(C2(C)CCCC2)c(O)cc1C)c1cc(C2(C)CCCC2)c(O)cc1C
Mol. weight [g/mol]:	462.71
CAS:	26292-67-1

Physical Properties

Property code	Value	Unit	Source
gf	131.10	kJ/mol	Joback Method
hf	-497.41	kJ/mol	Joback Method
hfus	44.28	kJ/mol	Joback Method
hvap	118.22	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	9.090		Crippen Method
mcvol	404.240	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
tb	1205.22	K	Joback Method
tc	1480.85	K	Joback Method
tf	824.32	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1658.67	J/molxK	1205.22	Joback Method
cpg	1715.49	J/molxK	1251.16	Joback Method
cpg	1777.62	J/molxK	1297.10	Joback Method
cpg	1845.75	J/molxK	1343.04	Joback Method
cpg	1920.59	J/molxK	1388.98	Joback Method
cpg	2002.82	J/molxK	1434.91	Joback Method
cpg	2093.16	J/molxK	1480.85	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=C26292671&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
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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