2,6-di-tert-Butyl-4-(dimethylaminomethyl)phenol

Other names:	Phenol, 4-[(dimethylamino)methyl]-2,6-bis(1,1-dimethylethyl)- p-Cresol, 2,6-di-tert-butyl-«alpha»-(dimethylamino)- Ethyl 703 N-(3,5-Di-tert-butyl-4-hydroxybenzyl)dimethylamine 2,6-Di-tert-butyl-«alpha»-(dimethylamino)-p-cresol Agidol 3 Ethyl antioxidant 703 F 1 OMI 2,6-Di-tert-butyl-alpha-dimethylamino-p-cresol 2,6-Di-t-butyl-4-(dimethylaminomethyl)phenol F 1 (Antioxidant) NSC 27823
Inchi:	InChI=1S/C17H29NO/c1-16(2,3)13-9-12(11-18(7)8)10-14(15(13)19)17(4,5)6/h9-10,19H,1
InchiKey:	VMZVBRIIHDRYGK-UHFFFAOYSA-N
Formula:	C17H29NO
SMILES:	CN(C)Cc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	263.42
CAS:	88-27-7

Physical Properties

Property code	Value	Unit	Source
gf	147.25	kJ/mol	Joback Method
hf	-307.90	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	69.50	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	4.049		Crippen Method
mcvol	242.480	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
tb	711.60	K	Joback Method
tc	927.62	K	Joback Method
tf	481.84	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.40	J/mol×K	711.60	Joback Method
cpg	728.95	J/mol×K	747.60	Joback Method
cpg	746.39	J/mol×K	783.61	Joback Method
cpg	762.83	J/mol×K	819.61	Joback Method
cpg	778.43	J/mol×K	855.62	Joback Method
cpg	793.31	J/mol×K	891.62	Joback Method
cpg	807.61	J/mol×K	927.62	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=C88277&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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