

Alpha,alpha-ethylenediimino-bis-(4-tert-butyl-o-cr

Inchi:	InChI=1S/C24H36N2O2/c1-23(2,3)19-7-9-21(27)17(13-19)15-25-11-12-26-16-18-14-20(2
InchiKey:	QKKQCRKTFAHWMC-UHFFFAOYSA-N
Formula:	C24H36N2O2
SMILES:	CC(C)(C)c1ccc(O)c(CNCCNCc2cc(C(C)(C)C)ccc2O)c1
Mol. weight [g/mol]:	384.55
CAS:	116373-76-3

Physical Properties

Property code	Value	Unit	Source
gf	231.98	kJ/mol	Joback Method
hf	-353.75	kJ/mol	Joback Method
hfus	52.16	kJ/mol	Joback Method
hvap	111.20	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.572		Crippen Method
mcvol	333.200	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
tb	1066.96	K	Joback Method
tc	1313.46	K	Joback Method
tf	771.72	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.29	J/molxK	1066.96	Joback Method
cpg	1191.72	J/molxK	1108.04	Joback Method
cpg	1213.78	J/molxK	1149.13	Joback Method
cpg	1236.76	J/molxK	1190.21	Joback Method
cpg	1260.95	J/molxK	1231.29	Joback Method
cpg	1286.64	J/molxK	1272.37	Joback Method
cpg	1314.14	J/molxK	1313.46	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=C116373763&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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