4,7-Methanobenzofuran, 2,2'-oxybis[octahydro-7,8,8-trimethyl-, [2«alpha»(2'R*,3'aS*,4'R*,7'R*,7'aS*),3a«alpha»,4«

Other names: (+)-Noe's reagent, (+)-MBF-OH dimer

Inchi: InChI=1S/C24H38O3/c1-21(2)15-7-9-23(21,5)19-13(15)11-17(26-19)25-18-12-14-16-8-1

InchiKey: VUDXCBLBKXFCNA-UHFFFAOYSA-N

Formula: C24H38O3

SMILES: CC1(C)C2CCC1(C)C1OC(OC3CC4C5CCC(C)(C4O3)C5(C)C)CC21

Mol. weight [g/mol]: 374.56

CAS: 81955-10-4

Physical Properties

Property code	Value	Unit	Source
gf	146.04	kJ/mol	Joback Method
hf	-571.51	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.378		Crippen Method
mcvol	301.470	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
tb	846.76	K	Joback Method
tc	1083.09	K	Joback Method
tf	606.37	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.65	J/mol×K	846.76	Joback Method
cpg	1158.18	J/mol×K	886.15	Joback Method
cpg	1193.29	J/mol×K	925.54	Joback Method
cpg	1230.65	J/mol×K	964.93	Joback Method
cpg	1270.88	J/mol×K	1004.31	Joback Method
cpg	1314.63	J/mol×K	1043.70	Joback Method
cpg	1362.56	J/mol×K	1083.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C81955104&Units=SI

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