2-([Bis(2-hydroxyethyl)amino]methyl)-4-tert-butyl

Inchi: InChI=1S/C15H25NO3/c1-15(2,3)13-4-5-14(19)12(10-13)11-16(6-8-17)7-9-18/h4-5,10,17
InchiKey: KUSJOXZZOOOPOD-UHFFFAOYSA-N
Formula: C15H25NO3
SMILES: CC(C)(C)c1ccc(O)c(CN(CCO)CCO)c1
Mol. weight [g/mol]: 267.36
CAS: 69470-50-4

Physical Properties

Property code	Value	Unit	Source
gf	-136.44	kJ/mol	Joback Method
hf	-550.86	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	99.04	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.476		Crippen Method
mcvol	226.040	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
tb	848.45	K	Joback Method
tc	1047.45	K	Joback Method
tf	566.00	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.81	J/mol×K	848.45	Joback Method
cpg	729.37	J/mol×K	881.62	Joback Method
cpg	741.44	J/mol×K	914.78	Joback Method
cpg	753.12	J/mol×K	947.95	Joback Method
cpg	764.50	J/mol×K	981.12	Joback Method
cpg	775.68	J/mol×K	1014.28	Joback Method
cpg	786.75	J/mol×K	1047.45	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=C69470504&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