Benzenamine, N,N-bis(2-hydroxy-3-phenoxypropyl)-

Other names: N,N-Bis(3-phenoxy-2-hydroxypropyl)aniline
Inchi: InChI=1S/C24H27NO4/c26-21(18-28-23-12-6-2-7-13-23)16-25(20-10-4-1-5-11-20)17-22(
InchiKey: PGJOBAKEAXXLSG-UHFFFAOYSA-N
Formula: C24H27NO4
SMILES: OC(COc1ccccc1)CN(CC(O)COc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 393.48
CAS: 3088-05-9

Physical Properties

Property code	Value	Unit	Source
chs	-12720.00 ± 4.20	kJ/mol	NIST Webbook
gf	110.69	kJ/mol	Joback Method
hf	-436.80 ± 4.20	kJ/mol	NIST Webbook
hfs	-582.80 ± 4.20	kJ/mol	NIST Webbook
hfus	46.57	kJ/mol	Joback Method
hvap	115.29	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.373		Crippen Method
mcvol	311.200	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
tb	1069.32	K	Joback Method
tc	1309.29	K	Joback Method
tf	608.07	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.00	J/mol×K	1229.30	Joback Method
cpg	1083.41	J/mol×K	1269.30	Joback Method
cpg	1037.62	J/mol×K	1069.32	Joback Method
cpg	1048.75	J/mol×K	1109.32	Joback Method
cpg	1058.78	J/mol×K	1149.31	Joback Method
cpg	1067.82	J/mol×K	1189.31	Joback Method

cpg	1090.19	J/mol×K	1309.29	Joback Method
hsubt	146.00 ± 4.20	kJ/mol	388.00	NIST Webbook
hvapt	131.00	kJ/mol	405.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3088059&Units=SI
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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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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