N,N-Bis(3-phenoxy-2-hydroxypropyl)butyl amine

Inchi: InChI=1S/C22H31NO4/c1-2-3-14-23(15-19(24)17-26-21-10-6-4-7-11-21)16-20(25)18-27-

InchiKey: ZDRJSLHBNGHXNK-UHFFFAOYSA-N

Formula: C22H31NO4

SMILES: CCCCN(CC(O)COc1ccccc1)CC(O)COc1ccccc1

Mol. weight [g/mol]: 373.49

CAS: 23257-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-18.56	kJ/mol	Joback Method
hf	-536.28	kJ/mol	Joback Method
hfus	47.34	kJ/mol	Joback Method
hvap	108.56	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	2.968		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
tb	996.88	K	Joback Method
tc	1220.51	K	Joback Method
tf	559.11	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.14	J/mol×K	1183.24	Joback Method
cpg	1029.57	J/mol×K	996.88	Joback Method
cpg	1042.88	J/mol×K	1034.15	Joback Method
cpg	1055.02	J/mol×K	1071.42	Joback Method
cpg	1066.06	J/mol×K	1108.70	Joback Method
cpg	1076.07	J/mol×K	1145.97	Joback Method
cpg	1093.34	J/mol×K	1220.51	Joback Method
hsubt	114.30	kJ/mol	387.00	NIST Webbook

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=C23257627&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
hsubt:	Enthalpy of sublimation at a given temperature
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