N-(3-Phenoxy-2-hydroxypropyl)-butylamine

Inchi: InChI=1S/C13H21NO2/c1-2-3-9-14-10-12(15)11-16-13-7-5-4-6-8-13/h4-8,12,14-15H,2-3,
InchiKey: JCLZQRQJFXFGGK-UHFFFAOYSA-N
Formula: C13H21NO2
SMILES: CCCCNCC(O)COc1ccccc1
Mol. weight [g/mol]: 223.31
CAS: 3246-04-6

Physical Properties

Property code	Value	Unit	Source
gf	16.12	kJ/mol	Joback Method
hf	-311.38	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	71.94	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.816		Crippen Method
mcvol	191.990	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
tb	687.85	K	Joback Method
tc	877.63	K	Joback Method
tf	383.40	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.44	J/mol×K	687.85	Joback Method
cpg	552.57	J/mol×K	719.48	Joback Method
cpg	565.90	J/mol×K	751.11	Joback Method
cpg	578.47	J/mol×K	782.74	Joback Method
cpg	590.30	J/mol×K	814.37	Joback Method
cpg	601.41	J/mol×K	846.00	Joback Method
cpg	611.83	J/mol×K	877.63	Joback Method
hsubt	133.90	kJ/mol	335.50	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=C3246046&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