2-Propanol, 1-phenoxy-3-(phenylamino)-

Other names: 1-Anilino-3-phenoxy-2-propanol
N-(3-Phenoxy-2-hydroxypropyl)aniline
Inchi: InChI=1S/C15H17NO2/c17-14(11-16-13-7-3-1-4-8-13)12-18-15-9-5-2-6-10-15/h1-10,14,1
InchiKey: DSXTWXWHWLDHFS-UHFFFAOYSA-N
Formula: C15H17NO2
SMILES: OC(CNc1ccccc1)COc1ccccc1
Mol. weight [g/mol]: 243.30
CAS: 16112-55-3

Physical Properties

Property code	Value	Unit	Source
chs	-8034.00 ± 3.00	kJ/mol	NIST Webbook
gf	145.37	kJ/mol	Joback Method
hf	-185.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-298.00 ± 3.00	kJ/mol	NIST Webbook
hfus	29.54	kJ/mol	Joback Method
hvap	78.67	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.538		Crippen Method
mcvol	196.410	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	760.29	K	Joback Method
tc	977.39	K	Joback Method
tf	432.36	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.44	J/mol×K	868.84	Joback Method
cpg	606.99	J/mol×K	905.02	Joback Method
cpg	616.69	J/mol×K	941.21	Joback Method
cpg	559.10	J/mol×K	760.29	Joback Method
cpg	572.54	J/mol×K	796.47	Joback Method

cpg	584.97	J/mol×K	832.66	Joback Method
cpg	625.57	J/mol×K	977.39	Joback Method
hsubt	113.90	kJ/mol	328.00	NIST Webbook
hsubt	114.00 ± 2.00	kJ/mol	343.00	NIST Webbook
hvapt	99.90	kJ/mol	358.00	NIST Webbook

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=C16112553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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