2-[(Dimethylamino)methyl]-4-(pentyloxy)phenol

Inchi: InChI=1S/C14H23NO2/c1-4-5-6-9-17-13-7-8-14(16)12(10-13)11-15(2)3/h7-8,10,16H,4-6,
InchiKey: BLRXKTDGVXXAER-UHFFFAOYSA-N
Formula: C14H23NO2
SMILES: CCCCCOc1ccc(O)c(CN(C)C)c1
Mol. weight [g/mol]: 237.34
CAS: 96933-86-7

Physical Properties

Property code	Value	Unit	Source
gf	20.94	kJ/mol	Joback Method
hf	-349.23	kJ/mol	Joback Method
hfus	35.66	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.023		Crippen Method
mcvol	206.080	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
tb	666.86	K	Joback Method
tc	868.10	K	Joback Method
tf	452.90	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.92	J/mol×K	666.86	Joback Method
cpg	587.00	J/mol×K	700.40	Joback Method
cpg	602.20	J/mol×K	733.94	Joback Method
cpg	616.58	J/mol×K	767.48	Joback Method
cpg	630.22	J/mol×K	801.02	Joback Method
cpg	643.16	J/mol×K	834.56	Joback Method
cpg	655.48	J/mol×K	868.10	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=C96933867&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