

2-[(Dimethylamino)methyl]-4-propoxyphenol

Inchi:	InChI=1S/C12H19NO2/c1-4-7-15-11-5-6-12(14)10(8-11)9-13(2)3/h5-6,8,14H,4,7,9H2,1-3
InchiKey:	VOGIILVNOKZNB-UHFFFAOYSA-N
Formula:	C12H19NO2
SMILES:	CCCOc1ccc(O)c(CN(C)C)c1
Mol. weight [g/mol]:	209.28

Physical Properties

Property code	Value	Unit	Source
gf	4.10	kJ/mol	Joback Method
hf	-307.95	kJ/mol	Joback Method
hfus	30.48	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.243		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	621.10	K	Joback Method
tc	828.04	K	Joback Method
tf	430.36	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.54	J/molxK	621.10	Joback Method
cpg	482.62	J/molxK	655.59	Joback Method
cpg	496.84	J/molxK	690.08	Joback Method
cpg	510.25	J/molxK	724.57	Joback Method
cpg	522.92	J/molxK	759.06	Joback Method
cpg	534.91	J/molxK	793.55	Joback Method
cpg	546.27	J/molxK	828.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=B6004844&Units=SI

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

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