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

Inchi: InChI=1S/C12H19NO2/c1-9(2)15-11-5-6-12(14)10(7-11)8-13(3)4/h5-7,9,14H,8H2,1-4H3
InchiKey: UBZQUTRAEUDDIN-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: CC(C)Oc1ccc(O)c(CN(C)C)c1
Mol. weight [g/mol]: 209.28
CAS: 116496-63-0

Physical Properties

Property code	Value	Unit	Source
gf	1.66	kJ/mol	Joback Method
hf	-313.23	kJ/mol	Joback Method
hfus	26.96	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.241		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	620.66	K	Joback Method
tc	831.69	K	Joback Method
tf	415.36	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.98	J/mol×K	620.66	Joback Method
cpg	483.41	J/mol×K	655.83	Joback Method
cpg	497.92	J/mol×K	691.00	Joback Method
cpg	511.59	J/mol×K	726.18	Joback Method
cpg	524.49	J/mol×K	761.35	Joback Method
cpg	536.66	J/mol×K	796.52	Joback Method
cpg	548.18	J/mol×K	831.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116496630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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