N-2-(1-hydroxy-3-methyl) butylbenzamide

Inchi: InChI=1S/C12H17NO2/c1-9(2)11(8-14)13-12(15)10-6-4-3-5-7-10/h3-7,9,11,14H,8H2,1-2
InchiKey: CPFYFTYVCYKOBY-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CC(C)C(CO)N=C(O)c1ccccc1
Mol. weight [g/mol]: 207.27
CAS: 92265-07-1

Physical Properties

Property code	Value	Unit	Source
hf	-297.07	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.008		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
tb	760.68	K	Joback Method
tc	962.16	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92265071&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

hf: Enthalpy of formation 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

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