Benzamide, 4-hydroxy, 2-(1-methylethyl), N,6-dimethyl

Inchi: InChI=1S/C12H17NO2/c1-7(2)10-6-9(14)5-8(3)11(10)12(15)13-4/h5-7,14H,1-4H3,(H,13,1

InchiKey: VDANDIZLSPNVPC-UHFFFAOYSA-N

Formula: C12H17NO2

SMILES: CNC(=O)c1c(C)cc(O)cc1C(C)C

Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	-53.28	kJ/mol	Joback Method
hf	-319.12	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	71.71	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.184		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1750.00		NIST Webbook
tb	694.82	K	Joback Method
tc	917.89	K	Joback Method
tf	475.77	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.74	J/mol×K	694.82	Joback Method
cpg	485.10	J/mol×K	732.00	Joback Method
cpg	497.68	J/mol×K	769.18	Joback Method
cpg	509.55	J/mol×K	806.35	Joback Method
cpg	520.77	J/mol×K	843.53	Joback Method
cpg	531.43	J/mol×K	880.71	Joback Method
cpg	541.60	J/mol×K	917.89	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R84548&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume