

Benzamide, 2-hydroxy, 4-(1-methylethyl), N,5-dimethyl

Inchi:	InChI=1S/C12H17NO2/c1-7(2)9-6-11(14)10(5-8(9)3)12(15)13-4/h5-7,14H,1-4H3,(H,13,15)
InchiKey:	JGINIQLUCAJCFN-UHFFFAOYSA-N
Formula:	C12H17NO2
SMILES:	CNC(=O)c1cc(C)c(C(C)C)cc1O
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	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	694.82	K	Joback Method
tc	917.89	K	Joback Method
tf	475.77	K	Joback Method
vc	0.601	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R84534&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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