Benzamide, n-phenacyl-

Inchi: InChI=1S/C15H13NO2/c17-14(12-7-3-1-4-8-12)11-16-15(18)13-9-5-2-6-10-13/h1-10H,11
InchiKey: MIJZKZQWQXKSPA-UHFFFAOYSA-N
Formula: C15H13NO2
SMILES: O=C(CN=C(O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 239.27
CAS: 4190-14-1

Physical Properties

Property code	Value	Unit	Source
hf	-72.25	kJ/mol	Joback Method
hvap	80.36	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.874		Crippen Method
mcvol	187.810	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
tb	818.57	K	Joback Method
tc	1055.79	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4190141&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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