N-Benzoylpiperidine

Other names:	Benzoic acid N-piperidide
	Benzoic acid piperidide
	Benzoylpiperidine
	LG 20104
	N-Benzoyl piperidine
	N-Benzoylpiperidin
	NSC 1992
	NSC 26344
	P 162
	Piperidine, 1-benzoyl-
	Protectine I
	R 162
	«alpha»-Repellin
Inchi:	InChI=1S/C12H15NO/c14-12(11-7-3-1-4-8-11)13-9-5-2-6-10-13/h1,3-4,7-8H,2,5-6,9-10H
InchiKey:	YXTROGRGRSPWKL-UHFFFAOYSA-N
Formula:	C12H15NO
SMILES:	O=C(c1ccccc1)N1CCCCC1
Mol. weight [g/mol]:	189.26

Physical Properties

Property code	Value	Unit	Source
af	0.4871		Cheméo Relay (1.0)
gf	143.47	kJ/mol	Cheméo Relay (1.0, beta)
hf	-117.15	kJ/mol	Cheméo Relay (1.0)
hvap	73.45	kJ/mol	Cheméo Relay (1.0)
ie	8.84	eV	Cheméo Relay (1.0)
log10ws	-1.98		Cheméo Relay (1.0)
logp	2.313		Crippen Method
mcvol	156.870	ml/mol	McGowan Method
pc	2659.42	kPa	Cheméo Relay (1.0, beta)
tb	593.12	K	Cheméo Relay (1.0)
tc	820.45	K	Cheméo Relay (1.0)
tf	317.86	K	Cheméo Relay (1.0)
vc	0.562	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C776750&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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