Benzamide, N-isopropyl-

Inchi: InChI=1S/C10H13NO/c1-8(2)11-10(12)9-6-4-3-5-7-9/h3-8H,1-2H3,(H,11,12)
InchiKey: INOVPKZAEASFME-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CC(C)N=C(O)c1ccccc1
Mol. weight [g/mol]: 163.22
CAS: 5440-69-7

Physical Properties

Property code	Value	Unit	Source
hf	-98.28	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.400		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
tb	623.18	K	Joback Method
tc	838.51	K	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=C5440697&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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