

(E)-1-Indan-1-ylethanone methoxime

Inchi: InChI=1S/C12H15NO/c1-9(13-14-2)11-8-7-10-5-3-4-6-12(10)11/h3-6,11H,7-8H2,1-2H3
InchiKey: VUBQDTAFTPOVIF-UHFFFAOYSA-N
Formula: C12H15NO
SMILES: CON=C(C)C1CCc2ccccc21
Mol. weight [g/mol]: 189.25

Physical Properties

Property code	Value	Unit	Source
hf	-52.94	kJ/mol	Joback Method
hvap	50.96	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.739		Crippen Method
mcvol	156.870	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	611.34	K	Joback Method
tc	845.86	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U373309&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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