

(E)-2-(4-Methoxyphenyl)ethan-2-one methoxime

Inchi: InChI=1S/C10H13NO2/c1-8(11-13-3)9-4-6-10(12-2)7-5-9/h4-7H,1-3H3
InchiKey: VWKUDUNDAJKGEU-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CON=C(C)c1ccc(OC)cc1
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
hf	-216.68	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.066		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	581.26	K	Joback Method
tc	805.13	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373223&Units=SI>
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>

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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