CHALCONE MEOX-1

Inchi: InChI=1S/C16H15NO/c1-18-17-16(15-10-6-3-7-11-15)13-12-14-8-4-2-5-9-14/h2-13H,1H3
InchiKey: XQTLKDRBVNIEJF-BNSYYMJASA-N
Formula: C16H15NO
SMILES: CON=C(C=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 237.30

Physical Properties

Property code	Value	Unit	Source
hf	156.92	kJ/mol	Joback Method
hvap	61.52	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.750		Crippen Method
mcvol	196.030	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	721.98	K	Joback Method
tc	976.28	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=R438812&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