Benzoic acid, 4-nitroso-, methyl ester

Inchi: InChI=1S/C8H7NO3/c1-12-8(10)6-2-4-7(9-11)5-3-6/h2-5H,1H3
InchiKey: CAFWWZWJFFJXTF-UHFFFAOYSA-N
Formula: C8H7NO3
SMILES: COC(=O)c1ccc(N=O)cc1
Mol. weight [g/mol]: 165.15
CAS: 13170-28-0

Physical Properties

Property code	Value	Unit	Source
hf	-396.38	kJ/mol	Joback Method
hvap	54.59	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.871		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	553.79	K	Joback Method
tc	769.99	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=C13170280&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature