Mordant Orange 1, O,O'-dimethyl-

Inchi: InChI=1S/C15H13N3O5/c1-22-14-8-5-11(9-13(14)15(19)23-2)17-16-10-3-6-12(7-4-10)18
InchiKey: DMRGBNPNEMDBKI-UHFFFAOYSA-N
Formula: C15H13N3O5
SMILES: COC(=O)c1cc(N=Nc2ccc([N+](=O)[O-])cc2)ccc1OC
Mol. weight [g/mol]: 315.28

Physical Properties

Property code	Value	Unit	Source
hf	-254.84	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.805		Crippen Method
mcvol	221.080	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2835.00		NIST Webbook
tb	1010.65	K	Joback Method
tc	1276.89	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374251&Units=SI
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

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