

Mordant yellow 12, N,N,O,O'-tetramethyl-

Inchi: InChI=1S/C17H19N3O3/c1-20(2)14-8-5-12(6-9-14)18-19-13-7-10-16(22-3)15(11-13)17(2)
InchiKey: YYMAFBWDYIHCBV-UHFFFAOYSA-N
Formula: C17H19N3O3
SMILES: COC(=O)c1cc(N=Nc2ccc(N(C)C)cc2)ccc1OC
Mol. weight [g/mol]: 313.35

Physical Properties

Property code	Value	Unit	Source
hf	-217.83	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.963		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2998.00		NIST Webbook
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tb	917.01	K	Joback Method
tc	1157.93	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=U374252&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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