Alizarin Yellow GG, O,O'-dimethyl-

Inchi: InChI=1S/C15H13N3O5/c1-22-14-7-6-11(9-13(14)15(19)23-2)17-16-10-4-3-5-12(8-10)18

InchiKey: ZVINFZLLAWAZOT-UHFFFAOYSA-N

Formula: C15H13N3O5

SMILES: COC(=O)c1cc(N=Nc2cccc([N+](=O)[O-])c2)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	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
tb	1010.65	K	Joback Method
tc	1276.89	K	Joback Method

Sources

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=U374253&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/119-842-5/Alizarin-Yellow-GG-O-O-dimethyl.pdf
Generated by Cheméo on 2024-04-28 03:06:58.283429227 +0000 UTC m=+16562867.204006561.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.