METHYL RED

Other names: Benzoic acid, 2-[[4-(dimethylamino)phenyl]azo]-
Methyl red, CI 13020
o-((p-(Dimethylamino)phenyl)azo)benzoic acid
o-Methyl red
p-(Dimethylamino)azobenzene-o-carboxylic acid
Benzoic acid, o-((p-(dimethylamino)phenyl)azo)-
C.I. Acid Red 2
C.I. 13020
2-((4-Dimethylamino)phenylazo)benzoic acid
2-Carboxy-4'-(dimethylamino)azobenzene
4-Dimethylamino-2'-carboxylazobenzene
4'-(Dimethylamino)azobenzene-2-carboxylic acid
Cerven kysela 2
Cerven methylova
2-[(p-Dimethylamino)phenyl]azobenzoic acid
NSC 215212

Inchi: InChI=1S/C15H15N3O2/c1-18(2)12-9-7-11(8-10-12)16-17-14-6-4-3-5-13(14)15(19)20/h3

InchiKey: CEQFOVLGLXCDCX-UHFFFAOYSA-N

Formula: C15H15N3O2

SMILES: CN(C)c1ccc(N=Nc2ccccc2C(=O)O)cc1

Mol. weight [g/mol]: 269.30

Physical Properties

Property code	Value	Unit	Source
hf	23.87	kJ/mol	Cheméo Relay (1.0)
ie	7.26	eV	Cheméo Relay (1.0)
log10ws	-3.98		Cheméo Relay (1.0)
logp	3.866		Crippen Method
mcvol	207.770	ml/mol	McGowan Method
tf	486.28	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C493527&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point