

Disperse orange 3

Inchi:	InChI=1S/C12H10N4O2/c13-9-1-3-10(4-2-9)14-15-11-5-7-12(8-6-11)16(17)18/h1-8H,13H
InchiKey:	UNBOSJFEZZJZLR-UHFFFAOYSA-N
Formula:	C12H10N4O2
SMILES:	<chem>Nc1ccc(N=Nc2ccc([N+](=O)[O-])cc2)cc1</chem>
Mol. weight [g/mol]:	242.24
CAS:	730-40-5

Physical Properties

Property code	Value	Unit	Source
hf	347.17	kJ/mol	Cheméo Relay (1.0)
hvap	106.99	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-4.19		Cheméo Relay (1.0)
logp	3.592		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
tb	663.77	K	Cheméo Relay (1.0)
tf	488.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

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

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<https://www.cheméo.com/cid/108-611-3/Disperse-orange-3.pdf>

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