P-phenylazo carbanilic acid, n-propyl ester

Inchi: InChI=1S/C16H17N3O2/c1-2-12-21-16(20)17-13-8-10-15(11-9-13)19-18-14-6-4-3-5-7-14
InchiKey: BXCWCIFEVVUAPJ-VHEBQXMUSA-N
Formula: C16H17N3O2
SMILES: CCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 283.33
CAS: 93311-68-3

Physical Properties

Property code	Value	Unit	Source
hf	-56.09	kJ/mol	Joback Method
hvap	78.69	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	5.060		Crippen Method
mcvol	221.860	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
tb	899.48	K	Joback Method
tc	1145.97	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93311683&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:
https://www.chemeo.com/cid/16-838-4/P-phenylazo-carbanilic-acid-n-propyl-ester.pdf
Generated by Cheméo on 2024-04-26 05:01:10.430525343 +0000 UTC m=+16396919.351102654.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.