P-phenylazo carbanilic acid, n-butyl ester

Inchi: InChI=1S/C17H19N3O2/c1-2-3-13-22-17(21)18-14-9-11-16(12-10-14)20-19-15-7-5-4-6-8
InchiKey: LQKYSTYAPQKETJ-FMQUCBEESA-N
Formula: C17H19N3O2
SMILES: CCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 297.35
CAS: 2678-88-8

Physical Properties

Property code	Value	Unit	Source
hf	-76.73	kJ/mol	Joback Method
hvap	80.91	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	5.451		Crippen Method
mcvol	235.950	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
tb	922.36	K	Joback Method
tc	1165.62	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2678888&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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