3-(Phenylazo)-2,4-pentanedione

Other names:	2,4-Pentanedione, 3-(phenylazo)-
	Phenyl-azo-acetylaceton
	3-(phenylazo)pentane-2,4-dione
Inchi:	InChI=1S/C11H12N2O2/c1-8(14)11(9(2)15)13-12-10-6-4-3-5-7-10/h3-7,11H,1-2H3
InchiKey:	KZPRCESDIPAEAE-UHFFFAOYSA-N
Formula:	C11H12N2O2
SMILES:	CC(=O)C(N=Nc1ccccc1)C(C)=O
Mol. weight [g/mol]:	204.23
CAS:	56276-49-4

Physical Properties

Property code	Value	Unit	Source
hf	-217.06	kJ/mol	Joback Method
hvap	62.13	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.317		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
tb	734.26	K	Joback Method
tc	977.09	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56276494&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