

Diacetamate

Other names:	Acetamide, N-[4-(acetoxy)phenyl]- p-Acetoxyacetanilide Acetaminophen acetate Acetanilide, 4'-hydroxy-, acetate (ester) Diacetamat N-Acetyl-4-aminophenyl acetate 4-Acetamidophenyl acetate 4-Acetoxyacetanilide 4-(Acetylamino)phenyl acetate Acetanilide, 4'-hydroxy-, acetate NSC 33893 NSC 6083 O-Acetylparacetamol N-[4-(acetoxy)phenyl] acetamide
Inchi:	InChI=1S/C10H11NO3/c1-7(12)11-9-3-5-10(6-4-9)14-8(2)13/h3-6H,1-2H3,(H,11,12)
InchiKey:	UJAOSPFULOFZRR-UHFFFAOYSA-N
Formula:	C10H11NO3
SMILES:	CC(=O)Oc1ccc(N=C(C)O)cc1
Mol. weight [g/mol]:	193.20
CAS:	2623-33-8

Physical Properties

Property code	Value	Unit	Source
hf	-349.27	kJ/mol	Joback Method
hvap	70.02	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.220		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	704.89	K	Joback Method
tc	920.98	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.97	kJ/mol	427.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623338&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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