

3',4'-Acetoxyliide

Other names:	N-Acetyl-3,4-xylidine 3,4-Dimethylacetanilide Acetamide, N-(3,4-dimethylphenyl)- 3',4'-Acetoxyliide 3',4'-Dimethylacetanilide 3,4-DMA N-(3,4-dimethylphenyl)acetamide
Inchi:	InChI=1S/C10H13NO/c1-7-4-5-10(6-8(7)2)11-9(3)12/h4-6H,1-3H3,(H,11,12)
InchiKey:	UAOIEEWQVAXCFY-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CC(=O)Nc1ccc(C)c(C)c1
Mol. weight [g/mol]:	163.22
CAS:	2198-54-1

Physical Properties

Property code	Value	Unit	Source
gf	86.94	kJ/mol	Joback Method
hf	-95.25	kJ/mol	Joback Method
hfus	21.62	kJ/mol	Joback Method
hvap	54.64	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.262		Crippen Method
mvol	139.550	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	568.88	K	Joback Method
tc	786.12	K	Joback Method
tf	356.51	K	Joback Method
vc	0.528	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.02	J/mol×K	568.88	Joback Method
cpg	336.31	J/mol×K	605.09	Joback Method

cpg	348.83	J/mol×K	641.29	Joback Method
cpg	360.60	J/mol×K	677.50	Joback Method
cpg	371.66	J/mol×K	713.70	Joback Method
cpg	382.02	J/mol×K	749.91	Joback Method
cpg	391.70	J/mol×K	786.12	Joback Method

Sources

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=C2198541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/63-735-6/3-4-Acetoxyliide.pdf>

Generated by Cheméo on 2024-04-27 19:20:33.65059246 +0000 UTC m=+16534882.571169777.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.