2',3'-Acetoxylidide

Inchi: InChI=1S/C10H13NO/c1-7-5-4-6-10(8(7)2)11-9(3)12/h4-6H,1-3H3,(H,11,12)
InchiKey: SRSHEJADOPNDDF-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CC(=O)Nc1cccc(C)c1C
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
af	0.5412		Cheméo Relay (1.0)
gf	86.94	kJ/mol	Joback Method
hf	-193.03	kJ/mol	Cheméo Relay (1.0)
hfus	21.62	kJ/mol	Joback Method
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-2.05		Cheméo Relay (1.0)
logp	2.262		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	549.51	K	Cheméo Relay (1.0)
tc	789.05	K	Cheméo Relay (1.0)
tf	355.66	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C134985&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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