Acetoxyacetamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C10H10FNO3/c1-7(13)15-6-10(14)12-9-5-3-2-4-8(9)11/h2-5H,6H2,1H3,(H,12,1
InchiKey: ACBRPOCVRODIGK-UHFFFAOYSA-N
Formula: C10H10FNO3
SMILES: CC(=O)OCC(=O)Nc1ccccc1F
Mol. weight [g/mol]: 211.19

Physical Properties

Property code	Value	Unit	Source
gf	-332.16	kJ/mol	Joback Method
hf	-524.69	kJ/mol	Joback Method
hfus	27.87	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.327		Crippen Method
mcvol	148.760	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1570.00		NIST Webbook
tb	639.46	K	Joback Method
tc	850.42	K	Joback Method
tf	416.74	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.31	J/mol×K	639.46	Joback Method
cpg	381.71	J/mol×K	674.62	Joback Method
cpg	392.37	J/mol×K	709.78	Joback Method
cpg	402.32	J/mol×K	744.94	Joback Method
cpg	411.56	J/mol×K	780.10	Joback Method
cpg	420.11	J/mol×K	815.26	Joback Method
cpg	427.98	J/mol×K	850.42	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=U308290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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