2',5'-DIFLUOROACETOPHENONE

Other names: 1-(2,5-difluorophenyl)ethan-1-one
2,5-Difluoroacetophenone
Ethanone, 1-(2,5-difluorophenyl)-
Inchi: InChI=1S/C8H6F2O/c1-5(11)7-4-6(9)2-3-8(7)10/h2-4H,1H3
InchiKey: HLAFIZUVVWJAKL-UHFFFAOYSA-N
Formula: C8H6F2O
SMILES: CC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 156.13

Physical Properties

Property code	Value	Unit	Source
hfus	17.50	kJ/mol	Joback Method
ie	9.39	eV	Cheméo Relay (1.0)
logp	2.167		Crippen Method
mcvol	104.930	ml/mol	McGowan Method
tb	460.47	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.37	J/mol×K	471.49	Joback Method
cpg	219.12	J/mol×K	505.05	Joback Method
cpg	228.36	J/mol×K	538.61	Joback Method
cpg	237.10	J/mol×K	572.17	Joback Method
cpg	245.36	J/mol×K	605.73	Joback Method
cpg	253.14	J/mol×K	639.29	Joback Method
cpg	260.45	J/mol×K	672.86	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=C1979368&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature