Ethanone, 1-(2,6-difluorophenyl)-

Other names:	Acetophenone, 2',6'-difluoro- 2',6'-Difluoroacetophenone 2,6-Difluoroacetophenone 1-(2,6-difluorophenyl)ethan-1-one
Inchi:	InChI=1S/C8H6F2O/c1-5(11)8-6(9)3-2-4-7(8)10/h2-4H,1H3
InchiKey:	VGIIILXIQLXVLC-UHFFFAOYSA-N
Formula:	C8H6F2O
SMILES:	CC(=O)c1c(F)cccc1F
Mol. weight [g/mol]:	156.13
CAS:	13670-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-408.91	kJ/mol	Joback Method
hf	-499.66	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	42.11	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.167		Crippen Method
mcvol	104.930	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	471.49	K	Joback Method
tc	672.86	K	Joback Method
tf	282.49	K	Joback Method
vc	0.417	m3/kmol	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.70	K	2.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13670990&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume