3,5-Difluoroacetophenone

Inchi: InChI=1S/C8H6F2O/c1-5(11)6-2-7(9)4-8(10)3-6/h2-4H,1H3
InchiKey: OXJLDNSPGPBDCP-UHFFFAOYSA-N
Formula: C8H6F2O
SMILES: CC(=O)c1cc(F)cc(F)c1
Mol. weight [g/mol]: 156.13
CAS: 123577-99-1

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123577991&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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