2,6-Difluorobutyrophenone

Inchi: InChI=1S/C10H10F2O/c1-2-4-9(13)10-7(11)5-3-6-8(10)12/h3,5-6H,2,4H2,1H3
InchiKey: MNDPYRXCTIANDJ-UHFFFAOYSA-N
Formula: C10H10F2O
SMILES: CCCC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 184.18
CAS: 95727-77-8

Physical Properties

Property code	Value	Unit	Source
gf	-392.07	kJ/mol	Joback Method
hf	-540.94	kJ/mol	Joback Method
hfus	22.68	kJ/mol	Joback Method
hvap	46.57	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.948		Crippen Method
mcvol	133.110	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	517.25	K	Joback Method
tc	713.39	K	Joback Method
tf	305.03	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.18	J/mol×K	517.25	Joback Method
cpg	305.09	J/mol×K	549.94	Joback Method
cpg	316.38	J/mol×K	582.63	Joback Method
cpg	327.07	J/mol×K	615.32	Joback Method
cpg	337.17	J/mol×K	648.01	Joback Method
cpg	346.71	J/mol×K	680.70	Joback Method
cpg	355.70	J/mol×K	713.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95727778&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