Acetophenone, 2,2-difluoro

Inchi: InChI=1S/C8H6F2O/c9-8(10)7(11)6-4-2-1-3-5-6/h1-5,8H
InchiKey: OLYKCPDTXVZOQF-UHFFFAOYSA-N
Formula: C8H6F2O
SMILES: O=C(c1ccccc1)C(F)F
Mol. weight [g/mol]: 156.13

Physical Properties

Property code	Value	Unit	Source
gf	-392.09	kJ/mol	Joback Method
hf	-482.00	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.134		Crippen Method
mcvol	104.930	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	959.00		NIST Webbook
tb	461.09	K	Joback Method
tc	664.50	K	Joback Method
tf	242.45	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.18	J/mol×K	461.09	Joback Method
cpg	220.13	J/mol×K	494.99	Joback Method
cpg	230.40	J/mol×K	528.89	Joback Method
cpg	240.02	J/mol×K	562.80	Joback Method
cpg	249.01	J/mol×K	596.70	Joback Method
cpg	257.41	J/mol×K	630.60	Joback Method
cpg	265.23	J/mol×K	664.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514966&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume