Acetophenone, 2,2,2,4'-tetrafluoro

Inchi: InChI=1S/C8H4F4O/c9-6-3-1-5(2-4-6)7(13)8(10,11)12/h1-4H
InchiKey: LUKLMXJAEKXROG-UHFFFAOYSA-N
Formula: C8H4F4O
SMILES: O=C(c1ccc(F)cc1)C(F)(F)F
Mol. weight [g/mol]: 192.11

Physical Properties

Property code	Value	Unit	Source
gf	-786.06	kJ/mol	Joback Method
hf	-889.16	kJ/mol	Joback Method
hfus	16.63	kJ/mol	Joback Method
hvap	38.52	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.571		Crippen Method
mcvol	108.470	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
tb	461.82	K	Joback Method
tc	653.60	K	Joback Method
tf	273.57	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.03	J/mol×K	461.82	Joback Method
cpg	239.23	J/mol×K	493.78	Joback Method
cpg	248.72	J/mol×K	525.75	Joback Method
cpg	257.55	J/mol×K	557.71	Joback Method
cpg	265.74	J/mol×K	589.67	Joback Method
cpg	273.33	J/mol×K	621.63	Joback Method
cpg	280.36	J/mol×K	653.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514951&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

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