

Methanone, (3-fluorophenyl)(4-fluorophenyl)-

Inchi:	InChI=1S/C13H8F2O/c14-11-6-4-9(5-7-11)13(16)10-2-1-3-12(15)8-10/h1-8H
InchiKey:	ZHUXSAKDWNNBCQ-UHFFFAOYSA-N
Formula:	C13H8F2O
SMILES:	O=C(c1ccc(F)cc1)c1cccc(F)c1
Mol. weight [g/mol]:	218.20
CAS:	345-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-254.40	kJ/mol	Joback Method
hf	-366.33	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.196		Crippen Method
mvol	151.620	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	612.57	K	Joback Method
tc	842.48	K	Joback Method
tf	365.26	K	Joback Method
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.92	J/mol×K	612.57	Joback Method
cpg	370.06	J/mol×K	650.89	Joback Method
cpg	382.19	J/mol×K	689.21	Joback Method
cpg	393.39	J/mol×K	727.52	Joback Method
cpg	403.68	J/mol×K	765.84	Joback Method
cpg	413.13	J/mol×K	804.16	Joback Method
cpg	421.79	J/mol×K	842.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C345711&Units=SI

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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