3'-FLUORO-4'-METHOXYACETOPHENONE

Other names:	1-(3-fluoro-4-methoxyphenyl)ethan-1-one
	3'-Fluoro-4'-methoxyacetophenone
	3-Fluoro-4-methoxyacetophenone
	Ethanone, 1-(3-fluoro-4-methoxyphenyl)-
Inchi:	InChI=1S/C9H9FO2/c1-6(11)7-3-4-9(12-2)8(10)5-7/h3-5H,1-2H3
InchiKey:	LQASUDVYVOFKNK-UHFFFAOYSA-N
Formula:	C9H9FO2
SMILES:	COc1ccc(C(C)=O)cc1F
Mol. weight [g/mol]:	168.17

Physical Properties

Property code	Value	Unit	Source
hfus	18.20	kJ/mol	Joback Method
hvap	68.52	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-2.22		Cheméo Relay (1.0)
logp	2.037		Crippen Method
mcvol	123.120	ml/mol	McGowan Method
tb	499.18	K	Cheméo Relay (1.0)
tf	334.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.31	J/mol×K	517.52	Joback Method
cpg	275.58	J/mol×K	552.10	Joback Method
cpg	286.31	J/mol×K	586.68	Joback Method
cpg	296.50	J/mol×K	621.26	Joback Method
cpg	306.15	J/mol×K	655.83	Joback Method
cpg	315.26	J/mol×K	690.41	Joback Method
cpg	323.85	J/mol×K	724.99	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.70	K	2.70	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C455914&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point