

Methanone, (2-fluorophenyl)[2-(methylamino)-5-nitrophenyl]-

Other names:	2'-Fluoro-2-methylamino-5-nitrobenzophenone 2-methylamino-5-nitro-2'-fluor-benzophenone 2-Methylamino-5-nitro-2'-fluorobenzophenone Benzophenone, 2'-fluoro-2-methylamino-5-nitro Flunitrazepam benzophenone
Inchi:	InChI=1S/C14H11FN2O3/c1-16-13-7-6-9(17(19)20)8-11(13)14(18)10-4-2-3-5-12(10)15/h
InchiKey:	GVXPKRIRHDCGY-UHFFFAOYSA-N
Formula:	C14H11FN2O3
SMILES:	CNc1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1F
Mol. weight [g/mol]:	274.25
CAS:	735-06-8

Physical Properties

Property code	Value	Unit	Source
gf	64.14	kJ/mol	Joback Method
hf	-159.62	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.007		Crippen Method
mcvol	191.340	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2338.00		NIST Webbook
rinpol	2383.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tb	843.17	K	Joback Method
tc	1095.55	K	Joback Method
tf	584.73	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.91	J/mol×K	843.17	Joback Method
cpg	549.90	J/mol×K	885.23	Joback Method
cpg	559.82	J/mol×K	927.30	Joback Method
cpg	568.73	J/mol×K	969.36	Joback Method
cpg	576.72	J/mol×K	1011.42	Joback Method
cpg	583.85	J/mol×K	1053.49	Joback Method
cpg	590.19	J/mol×K	1095.55	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=C735068&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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