

2'-FLUOROACETANILIDE

Other names:	2'-Fluoroacetanilide N-(2-fluorophenyl)acetamide
Inchi:	InChI=1S/C8H8FNO/c1-6(11)10-8-5-3-2-4-7(8)9/h2-5H,1H3,(H,10,11)
InchiKey:	AUZPZBPZWHEIDY-UHFFFAOYSA-N
Formula:	C8H8FNO
SMILES:	CC(=O)Nc1ccccc1F
Mol. weight [g/mol]:	153.16

Physical Properties

Property code	Value	Unit	Source
hfus	19.91	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
ie	8.27 ± 0.03	eV	NIST Webbook
log10ws	-1.43		Cheméo Relay (1.0)
logp	1.784		Crippen Method
mcvol	113.140	ml/mol	McGowan Method
tb	507.18	K	Cheméo Relay (1.0)
tf	320.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.65	J/mol×K	517.41	Joback Method
cpg	253.72	J/mol×K	552.81	Joback Method
cpg	264.12	J/mol×K	588.21	Joback Method
cpg	273.86	J/mol×K	623.61	Joback Method
cpg	282.97	J/mol×K	659.01	Joback Method
cpg	291.48	J/mol×K	694.41	Joback Method
cpg	299.41	J/mol×K	729.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.20	K	1.90	NIST Webbook
tbrp	414.00 ± 1.00	K	1.90	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C399315&Units=SI
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
hfus:	Enthalpy of fusion 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

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