

# Acetamide, n,n'-(4,6-difluoro-2-nitro-m-phenylene)bis-

Inchi:	InChI=1S/C10H9F2N3O4/c1-4(16)13-8-6(11)3-7(12)9(14-5(2)17)10(8)15(18)19/h3H,1-2H
InchiKey:	HGPVHQIKZLZGBE-UHFFFAOYSA-N
Formula:	C10H9F2N3O4
SMILES:	CC(=O)Nc1c(F)cc(F)c(NC(C)=O)c1[N+](=O)[O-]
Mol. weight [g/mol]:	273.19
CAS:	4140-70-9

## Physical Properties

Property code	Value	Unit	Source
gf	-325.92	kJ/mol	Joback Method
hf	-580.28	kJ/mol	Joback Method
hfus	45.06	kJ/mol	Joback Method
hvap	84.10	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	1.790		Crippen Method
mcvol	172.060	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
tb	833.26	K	Joback Method
tc	1059.27	K	Joback Method
tf	628.93	K	Joback Method
vc	0.688	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.31	J/molxK	833.26	Joback Method
cpg	492.96	J/molxK	870.93	Joback Method
cpg	500.82	J/molxK	908.60	Joback Method
cpg	507.91	J/molxK	946.27	Joback Method
cpg	514.25	J/molxK	983.93	Joback Method
cpg	519.88	J/molxK	1021.60	Joback Method
cpg	524.80	J/molxK	1059.27	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4140709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4140709&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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