

# Fentiazac

<b>Inchi:</b>	InChI=1S/C17H14ClNO2S/c18-13-8-6-11(7-9-13)16-14(10-15(20)21)22-17(19-16)12-4-2
<b>InchiKey:</b>	YPGAFANIBNLVJH-UHFFFAOYSA-N
<b>Formula:</b>	C17H14ClNO2S
<b>SMILES:</b>	O=C(O)CC1SC(c2ccccc2)N=C1c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	331.82
<b>CAS:</b>	18046-21-4

## Physical Properties

Property code	Value	Unit	Source
gf	235.59	kJ/mol	Joback Method
hf	-10.49	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	99.38	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.418		Crippen Method
mvol	233.720	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	946.46	K	Joback Method
tc	1203.98	K	Joback Method
tf	662.31	K	Joback Method
vc	0.867	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.99	J/molxK	946.46	Joback Method
cpg	706.46	J/molxK	989.38	Joback Method
cpg	715.55	J/molxK	1032.30	Joback Method
cpg	723.34	J/molxK	1075.22	Joback Method
cpg	729.92	J/molxK	1118.14	Joback Method
cpg	735.35	J/molxK	1161.06	Joback Method
cpg	739.72	J/molxK	1203.98	Joback Method

# Sources

<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=C18046214&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18046214&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

# 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>hvap:</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<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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