

# (S)-Desmethylocitalopram

<b>Inchi:</b>	InChI=1S/C19H19FN2O/c1-22-10-2-9-19(16-4-6-17(20)7-5-16)18-8-3-14(12-21)11-15(18)
<b>InchiKey:</b>	PTJADDMMFYXMMG-LJQANCHMSA-N
<b>Formula:</b>	C19H19FN2O
<b>SMILES:</b>	CNCCCC1(c2ccc(F)cc2)OCc2cc(C#N)ccc21
<b>Mol. weight [g/mol]:</b>	310.37
<b>CAS:</b>	144025-14-9

## Physical Properties

Property code	Value	Unit	Source
gf	301.93	kJ/mol	Joback Method
hf	-18.56	kJ/mol	Joback Method
hfus	41.38	kJ/mol	Joback Method
hvap	83.80	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.471		Crippen Method
mcvol	239.190	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2508.30		NIST Webbook
tb	887.87	K	Joback Method
tc	1126.20	K	Joback Method
tf	580.94	K	Joback Method
vc	0.939	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.51	J/molxK	887.87	Joback Method
cpg	750.72	J/molxK	927.59	Joback Method
cpg	766.93	J/molxK	967.31	Joback Method
cpg	783.34	J/molxK	1007.03	Joback Method
cpg	800.19	J/molxK	1046.75	Joback Method
cpg	817.70	J/molxK	1086.47	Joback Method
cpg	836.08	J/molxK	1126.20	Joback Method

# Sources

<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=C144025149&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C144025149&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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