

Citalopram, bis-nor, acetyl

Inchi:	InChI=1S/C20H19FN2O2/c1-14(24)23-10-2-9-20(17-4-6-18(21)7-5-17)19-8-3-15(12-22)1
InchiKey:	MJXCQDCWTBXXPG-UHFFFAOYSA-N
Formula:	C20H19FN2O2
SMILES:	CC(=O)NCCCC1(c2ccc(F)cc2)OCc2cc(C#N)ccc21
Mol. weight [g/mol]:	338.38

Physical Properties

Property code	Value	Unit	Source
gf	181.43	kJ/mol	Joback Method
hf	-151.78	kJ/mol	Joback Method
hfus	45.57	kJ/mol	Joback Method
hvap	92.77	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.387		Crippen Method
mvol	254.850	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	964.62	K	Joback Method
tc	1206.15	K	Joback Method
tf	642.14	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.25	J/molxK	964.62	Joback Method
cpg	823.07	J/molxK	1004.88	Joback Method
cpg	840.24	J/molxK	1045.13	Joback Method
cpg	857.98	J/molxK	1085.39	Joback Method
cpg	876.53	J/molxK	1125.64	Joback Method
cpg	896.12	J/molxK	1165.90	Joback Method
cpg	916.98	J/molxK	1206.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R195916&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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