Citalopram, nor, acetyl

Inchi: InChI=1S/C21H21FN2O2/c1-15(25)24(2)11-3-10-21(18-5-7-19(22)8-6-18)20-9-4-16(13-2
InchiKey: XSYWUOFETHDSCD-UHFFFAOYSA-N
Formula: C21H21FN2O2
SMILES: CC(=O)N(C)CCCC1(c2ccc(F)cc2)OCc2cc(C#N)ccc21
Mol. weight [g/mol]: 352.40

Physical Properties

Property code	Value	Unit	Source
gf	211.24	kJ/mol	Joback Method
hf	-158.36	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	90.60	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	3.730		Crippen Method
mcvol	268.940	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2820.00		NIST Webbook
tb	949.77	K	Joback Method
tc	1187.01	K	Joback Method
tf	633.22	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.69	J/mol×K	949.77	Joback Method
cpg	869.03	J/mol×K	989.31	Joback Method
cpg	886.61	J/mol×K	1028.85	Joback Method
cpg	904.66	J/mol×K	1068.39	Joback Method
cpg	923.41	J/mol×K	1107.93	Joback Method
cpg	943.11	J/mol×K	1147.47	Joback Method
cpg	963.97	J/mol×K	1187.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R195921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume