Fluoxetin (carbinol), diacetyl

Inchi: InChI=1S/C14H19NO3/c1-11(16)15(3)10-9-14(18-12(2)17)13-7-5-4-6-8-13/h4-8,14H,9-1
InchiKey: QRRGVEBZOSRDKR-UHFFFAOYSA-N
Formula: C14H19NO3
SMILES: CC(=O)OC(CCN(C)C(C)=O)c1ccccc1
Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-75.09	kJ/mol	Joback Method
hf	-390.89	kJ/mol	Joback Method
hfus	29.94	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.159		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	688.56	K	Joback Method
tc	896.60	K	Joback Method
tf	413.52	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.69	J/mol×K	688.56	Joback Method
cpg	569.03	J/mol×K	723.23	Joback Method
cpg	583.37	J/mol×K	757.91	Joback Method
cpg	596.72	J/mol×K	792.58	Joback Method
cpg	609.13	J/mol×K	827.26	Joback Method
cpg	620.64	J/mol×K	861.93	Joback Method
cpg	631.27	J/mol×K	896.60	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=R195956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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