Fluoxetin, nor (carbinol), diacetyl

Inchi: InChI=1S/C13H17NO3/c1-10(15)14-9-8-13(17-11(2)16)12-6-4-3-5-7-12/h3-7,13H,8-9H2,
InchiKey: KCPKAURIPUCAGX-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: CC(=O)NCCC(OC(C)=O)c1ccccc1
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-104.90	kJ/mol	Joback Method
hf	-384.31	kJ/mol	Joback Method
hfus	29.43	kJ/mol	Joback Method
hvap	68.76	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.817		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	703.41	K	Joback Method
tc	916.73	K	Joback Method
tf	422.44	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.47	J/mol×K	703.41	Joback Method
cpg	529.58	J/mol×K	738.96	Joback Method
cpg	542.73	J/mol×K	774.52	Joback Method
cpg	554.94	J/mol×K	810.07	Joback Method
cpg	566.24	J/mol×K	845.63	Joback Method
cpg	576.66	J/mol×K	881.18	Joback Method
cpg	586.23	J/mol×K	916.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R195976&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