Venlafaxine-M (O-desmethyl-HO-) isomer-1 2AC

Inchi: InChI=1S/C21H31NO5/c1-15(23)26-20-13-17(9-10-19(20)25-5)18(14-22(3)4)21(27-16(2)
InchiKey: QJSZAROWHJCRJN-UHFFFAOYSA-N
Formula: C21H31NO5
SMILES: COc1ccc(C(CN(C)C)C2(OC(C)=O)CCCCC2)cc1OC(C)=O
Mol. weight [g/mol]: 377.47

Physical Properties

Property code	Value	Unit	Source
gf	-226.45	kJ/mol	Joback Method
hf	-753.19	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	87.59	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.532		Crippen Method
mcvol	302.860	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
tb	923.31	K	Joback Method
tc	1147.93	K	Joback Method
tf	593.19	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.29	J/mol×K	923.31	Joback Method
cpg	1023.44	J/mol×K	960.75	Joback Method
cpg	1041.77	J/mol×K	998.18	Joback Method
cpg	1059.41	J/mol×K	1035.62	Joback Method
cpg	1076.47	J/mol×K	1073.05	Joback Method
cpg	1093.08	J/mol×K	1110.49	Joback Method
cpg	1109.35	J/mol×K	1147.93	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331256&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
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