Venlafaxine-M (O-desmethyl-) 2AC

Inchi: InChI=1S/C20H29NO4/c1-15(22)24-18-10-8-17(9-11-18)19(14-21(3)4)20(25-16(2)23)12-
InchiKey: FJPCUDTUEULBNQ-UHFFFAOYSA-N
Formula: C20H29NO4
SMILES: CC(=O)Oc1ccc(C(CN(C)C)C2(OC(C)=O)CCCCC2)cc1
Mol. weight [g/mol]: 347.45

Physical Properties

Property code	Value	Unit	Source
gf	-120.24	kJ/mol	Joback Method
hf	-588.86	kJ/mol	Joback Method
hfus	31.82	kJ/mol	Joback Method
hvap	82.30	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.523		Crippen Method
mcvol	282.900	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2230.00		NIST Webbook
tb	873.03	K	Joback Method
tc	1098.57	K	Joback Method
tf	547.17	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.25	J/mol×K	873.03	Joback Method
cpg	932.58	J/mol×K	910.62	Joback Method
cpg	951.12	J/mol×K	948.21	Joback Method
cpg	968.98	J/mol×K	985.80	Joback Method
cpg	986.33	J/mol×K	1023.39	Joback Method
cpg	1003.30	J/mol×K	1060.98	Joback Method
cpg	1020.03	J/mol×K	1098.57	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=R331241&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