Doxepin M(HO), acetylated, isomer # 1

Inchi: InChI=1S/C21H23NO3/c1-15(23)25-20-12-6-10-19-18(11-7-13-22(2)3)17-9-5-4-8-16(17)
InchiKey: KXTVPIGPNLBPMJ-WQRHYEAKSA-N
Formula: C21H23NO3
SMILES: CC(=O)Oc1cccc2c1OCc1ccccc1C2=CCCN(C)C
Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
gf	226.53	kJ/mol	Joback Method
hf	-178.22	kJ/mol	Joback Method
hfus	48.23	kJ/mol	Joback Method
hvap	85.60	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	3.888		Crippen Method
mcvol	267.360	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2540.00		NIST Webbook
tb	881.91	K	Joback Method
tc	1112.34	K	Joback Method
tf	580.57	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.40	J/mol×K	881.91	Joback Method
cpg	832.50	J/mol×K	920.31	Joback Method
cpg	846.59	J/mol×K	958.72	Joback Method
cpg	859.78	J/mol×K	997.12	Joback Method
cpg	872.17	J/mol×K	1035.53	Joback Method
cpg	883.86	J/mol×K	1073.93	Joback Method
cpg	894.97	J/mol×K	1112.34	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=R310888&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