Doxepin M(Nor-HO), diacetylated, isomer # 1

Inchi: InChI=1S/C22H23NO4/c1-15(24)23(3)13-7-11-19-18-9-5-4-8-17(18)14-26-22-20(19)10-6

InchiKey: KTFIZIRUAOKHNH-ODLFYWEKSA-N

Formula: C22H23NO4

SMILES: CC(=O)Oc1cccc2c1OCc1ccccc1C2=CCCN(C)C(C)=O

Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	106.03	kJ/mol	Joback Method
hf	-311.44	kJ/mol	Joback Method
hfus	52.42	kJ/mol	Joback Method
hvap	94.57	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.804		Crippen Method
mcvol	283.020	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2987.00		NIST Webbook
tb	958.66	K	Joback Method
tc	1193.60	K	Joback Method
tf	641.77	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.96	J/mol×K	958.66	Joback Method
cpg	900.61	J/mol×K	997.82	Joback Method
cpg	913.35	J/mol×K	1036.97	Joback Method
cpg	925.28	J/mol×K	1076.13	Joback Method
cpg	936.53	J/mol×K	1115.29	Joback Method
cpg	947.21	J/mol×K	1154.45	Joback Method
cpg	957.42	J/mol×K	1193.60	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=R310902&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