

2,5-Dimethoxy-4-methyl-«beta»-phenethylamine-N-(O-desmethyl-desamino-COOH-), methyl-acetylated, I

SMILES: COC(=O)Cc1cc(OC(C)=O)c(C)cc1OC

Mol. weight [g/mol]: 252.26

Physical Properties

Property code	Value	Unit	Source
gf	-430.74	kJ/mol	Joback Method
hf	-731.35	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.644		Crippen Method
mcvol	191.020	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	713.46	K	Joback Method
tc	921.93	K	Joback Method
tf	466.80	K	Joback Method
vc	0.722	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.45	J/molxK	713.46	Joback Method
cpg	569.95	J/molxK	887.19	Joback Method
cpg	559.98	J/molxK	852.44	Joback Method
cpg	549.13	J/molxK	817.70	Joback Method
cpg	537.41	J/molxK	782.95	Joback Method
cpg	524.84	J/molxK	748.21	Joback Method
cpg	579.00	J/molxK	921.93	Joback Method
dvisc	0.0001036	Paxs	713.46	Joback Method

dvisc	0.0001259	Paxs	672.35	Joback Method
dvisc	0.0001569	Paxs	631.24	Joback Method
dvisc	0.0002016	Paxs	590.13	Joback Method
dvisc	0.0002690	Paxs	549.02	Joback Method
dvisc	0.0003761	Paxs	507.91	Joback Method
dvisc	0.0005577	Paxs	466.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438312&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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