

2,5-Dimethoxy-4-methyl-«beta»-phenethylamine-M (desamino-COOH-), methyl

InChI: COC(=O)C(C)C(C)C(OC)C1=CC=C(C=C1)OC
InChIKey: QESMEYPKJZIRRH-UHFFFAOYSA-N
Formula: C12H16O4
SMILES: COC(=O)C(C)C(C)C(OC)c(C)cc1OC
Mol. weight [g/mol]: 224.25

Physical Properties

Property code	Value	Unit	Source
gf	-310.24	kJ/mol	Joback Method
hf	-598.13	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	60.54	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.728		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1760.00		NIST Webbook
tb	636.71	K	Joback Method
tc	841.45	K	Joback Method
tf	405.60	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.68	J/molxK	636.71	Joback Method
cpg	506.94	J/molxK	807.33	Joback Method
cpg	495.73	J/molxK	773.20	Joback Method
cpg	483.78	J/molxK	739.08	Joback Method
cpg	471.10	J/molxK	704.96	Joback Method
cpg	457.73	J/molxK	670.83	Joback Method
cpg	517.39	J/molxK	841.45	Joback Method
dvisc	0.0001124	Paxs	636.71	Joback Method
dvisc	0.0001367	Paxs	598.19	Joback Method

dvisc	0.0001707	Paxs	559.67	Joback Method
dvisc	0.0002204	Paxs	521.15	Joback Method
dvisc	0.0002963	Paxs	482.64	Joback Method
dvisc	0.0004193	Paxs	444.12	Joback Method
dvisc	0.0006338	Paxs	405.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438243&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

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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