

Ramipril desethyl 3Me (Ramiprilate 3Me)

Inchi: InChI=1S/C25H35NO5/c1-16(23(27)22-19-12-8-11-18(19)15-20(22)24(28)30-3)26(2)21(2)
InchiKey: ONQATEOHSCLCLEF-SLMGIOGOSA-N
Formula: C25H35NO5
SMILES: COC(=O)C1CC2CCCC2C1C(=O)C(C)N(C)C(Cc1ccccc1)C(=O)OC
Mol. weight [g/mol]: 429.55

Physical Properties

Property code	Value	Unit	Source
gf	-136.95	kJ/mol	Joback Method
hf	-775.41	kJ/mol	Joback Method
hfus	51.91	kJ/mol	Joback Method
hvap	99.40	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.276		Crippen Method
mvol	344.060	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	1028.77	K	Joback Method
tc	1262.90	K	Joback Method
tf	615.01	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1222.47	J/molxK	1028.77	Joback Method
cpg	1237.85	J/molxK	1067.79	Joback Method
cpg	1251.69	J/molxK	1106.81	Joback Method
cpg	1264.11	J/molxK	1145.84	Joback Method
cpg	1275.20	J/molxK	1184.86	Joback Method
cpg	1285.07	J/molxK	1223.88	Joback Method
cpg	1293.83	J/molxK	1262.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R549987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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