R,S-N-methyl-1-(2-methoxyphenyl)-2-aminopropa (bis-desmethyl-methoxy-), 2AC

InChI: InChI=1S/C13H17NO3/c1-9(14-10(2)15)8-12-6-4-5-7-13(12)17-11(3)16/h4-7,9H,8H2,1-3

InChIKey: WRQHUEKGFQVNQN-UHFFFAOYSA-N

Formula: C13H17NO3

SMILES: CC(=O)NC(C)Cc1ccccc1OC(C)=O

Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-114.53	kJ/mol	Joback Method
hf	-395.78	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	69.42	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	1.679		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook
tb	708.39	K	Joback Method
tc	922.53	K	Joback Method
tf	434.96	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.46	J/mol×K	708.39	Joback Method
cpg	528.43	J/mol×K	744.08	Joback Method
cpg	541.47	J/mol×K	779.77	Joback Method
cpg	553.59	J/mol×K	815.46	Joback Method
cpg	564.81	J/mol×K	851.15	Joback Method
cpg	575.15	J/mol×K	886.84	Joback Method
cpg	584.64	J/mol×K	922.53	Joback Method

Sources

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=R290967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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