R,S-N-methyl-1-(2-methoxyphenyl)-2-aminopropa
(O-demethyl-methyoxy-), isomer 2, 2AC

Inchi: InChI=1S/C15H21NO4/c1-10(16-4)11(2)17)9-13-7-6-8-14(19-5)15(13)20-12(3)18/h6-8,10
InchiKey: WKZYGGDDATZFAF-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: COc1cccc(CC(C)N(C)C(C)=O)c1OC(C)=O
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-190.93	kJ/mol	Joback Method
hf	-566.69	kJ/mol	Joback Method
hfus	32.94	kJ/mol	Joback Method
hvap	72.55	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.030		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2115.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	743.82	K	Joback Method
tc	949.44	K	Joback Method
tf	472.06	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.37	J/mol×K	743.82	Joback Method
cpg	648.40	J/mol×K	778.09	Joback Method
cpg	662.44	J/mol×K	812.36	Joback Method
cpg	675.49	J/mol×K	846.63	Joback Method
cpg	687.57	J/mol×K	880.90	Joback Method
cpg	698.69	J/mol×K	915.17	Joback Method
cpg	708.87	J/mol×K	949.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R290992&Units=SI

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