R,S-N-methyl-1-(2-methoxyphenyl)-2-aminopropa
(O-demethyl-OH-alkyl-); (threo); 3AC

Inchi: InChI=1S/C16H21NO5/c1-10(17-15(21)11(2)18)16(22-13(4)20)14-8-6-7-9-15(14)21-12(3)19/h

InchiKey: YZXUVOKUPJYXOC-UHFFFAOYSA-N

Formula: C16H21NO5

SMILES: CC(=O)Oc1ccccc1C(OC(C)=O)C(C)N(C)C(C)=O

Mol. weight [g/mol]: 307.34

Physical Properties

Property code	Value	Unit	Source
gf	-304.24	kJ/mol	Joback Method
hf	-693.72	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	80.47	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.083		Crippen Method
mcvol	238.970	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	815.15	K	Joback Method
tc	1027.54	K	Joback Method
tf	505.74	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.30	J/mol×K	815.15	Joback Method
cpg	720.13	J/mol×K	850.55	Joback Method
cpg	732.84	J/mol×K	885.95	Joback Method
cpg	744.44	J/mol×K	921.34	Joback Method
cpg	754.96	J/mol×K	956.74	Joback Method
cpg	764.42	J/mol×K	992.14	Joback Method
cpg	772.84	J/mol×K	1027.54	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=R291004&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