R,S-N-methyl-1-(2-methoxyphenyl)-2-aminopropan (O-demethyl-HO-aryl-), 3AC

Inchi: InChI=1S/C16H21NO5/c1-10(17(5)11(2)18)8-14-9-15(21-12(3)19)6-7-16(14)22-13(4)20/h
InchiKey: SMRJGNPFZITSMB-UHFFFAOYSA-N
Formula: C16H21NO5
SMILES: CC(=O)Oc1ccc(OC(C)=O)c(CC(C)N(C)C(C)=O)c1
Mol. weight [g/mol]: 307.34

Physical Properties

Property code	Value	Unit	Source
gf	-311.43	kJ/mol	Joback Method
hf	-699.91	kJ/mol	Joback Method
hfus	37.13	kJ/mol	Joback Method
hvap	81.52	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	1.947		Crippen Method
mcvol	238.970	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2190.00		NIST Webbook
tb	820.57	K	Joback Method
tc	1031.04	K	Joback Method
tf	533.26	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.62	J/mol×K	820.57	Joback Method
cpg	718.19	J/mol×K	855.65	Joback Method
cpg	730.68	J/mol×K	890.73	Joback Method
cpg	742.10	J/mol×K	925.80	Joback Method
cpg	752.47	J/mol×K	960.88	Joback Method
cpg	761.79	J/mol×K	995.96	Joback Method
cpg	770.09	J/mol×K	1031.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R290972&Units=SI
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

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

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