

Merresectine A

Inchi: InChI=1S/C15H19NO3/c1-18-13-4-2-3-10(7-13)15(17)19-14-8-11-5-6-12(9-14)16-11/h2-
InchiKey: GWVGSKHJYDCEQ-IMRBUKKESA-N
Formula: C15H19NO3
SMILES: COc1cccc(C(=O)OC2CC3CCC(C2)N3)c1
Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
gf	16.58	kJ/mol	Joback Method
hf	-354.14	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	70.11	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.135		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinsol	2195.00		NIST Webbook
tb	738.87	K	Joback Method
tc	976.84	K	Joback Method
tf	521.77	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.10	J/mol×K	738.87	Joback Method
cpg	620.50	J/mol×K	778.53	Joback Method
cpg	637.49	J/mol×K	818.19	Joback Method
cpg	653.11	J/mol×K	857.85	Joback Method
cpg	667.41	J/mol×K	897.52	Joback Method
cpg	680.43	J/mol×K	937.18	Joback Method
cpg	692.22	J/mol×K	976.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R510068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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