(-)-Jasmonic acid, (S)-Asp conjugate, methyl ester

Inchi: InChI=1S/C17H26N2O5/c1-3-4-5-6-12-11(7-8-14(12)20)9-16(22)19-13(10-15(18)21)17(2

InchiKey: WFVJNNZQFWYNPU-VAFQMXCQSA-N

Formula: C17H26N2O5

SMILES: CCC=CCC1C(=O)CCC1CC(=O)NC(CC(N)=O)C(=O)OC

Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-259.63	kJ/mol	Joback Method
hf	-762.53	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	96.93	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	0.861		Crippen Method
mcvol	267.340	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2427.00		NIST Webbook
tb	977.24	K	Joback Method
tc	1205.65	K	Joback Method
tf	644.09	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.32	J/mol×K	977.24	Joback Method
cpg	918.59	J/mol×K	1015.31	Joback Method
cpg	929.38	J/mol×K	1053.38	Joback Method
cpg	938.71	J/mol×K	1091.45	Joback Method
cpg	946.62	J/mol×K	1129.51	Joback Method
cpg	953.13	J/mol×K	1167.58	Joback Method
cpg	958.26	J/mol×K	1205.65	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=R169630&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