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

Inchi: InChI=1S/C22H29NO4/c1-3-4-6-11-18-17(12-13-20(18)24)15-21(25)23-19(22(26)27-2)14

InchiKey: JFDVKJZZXXFJEY-DYCGSOJJSA-N

Formula: C22H29NO4

SMILES: CCC=CCC1C(=O)CCC1CC(=O)NC(Cc1ccccc1)C(=O)OC

Mol. weight [g/mol]: 371.47

Physical Properties

Property code	Value	Unit	Source
gf	-42.65	kJ/mol	Joback Method
hf	-550.41	kJ/mol	Joback Method
hfus	47.46	kJ/mol	Joback Method
hvap	92.94	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.229		Crippen Method
mcvol	302.480	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2716.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	991.92	K	Joback Method
tc	1225.51	K	Joback Method
tf	593.67	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.23	J/mol×K	991.92	Joback Method
cpg	1039.26	J/mol×K	1030.85	Joback Method
cpg	1051.69	J/mol×K	1069.78	Joback Method
cpg	1062.58	J/mol×K	1108.72	Joback Method
cpg	1071.98	J/mol×K	1147.65	Joback Method
cpg	1079.95	J/mol×K	1186.58	Joback Method
cpg	1086.55	J/mol×K	1225.51	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=R169670&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