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

Inchi: InChI=1S/C18H27NO6/c1-4-5-6-7-13-12(8-9-15(13)20)10-16(21)19-14(18(23)25-3)11-17

InchiKey: GWLPBQMHLOWLFI-LFMXXEDNSA-N

Formula: C18H27NO6

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

Mol. weight [g/mol]: 353.41

Physical Properties

Property code	Value	Unit	Source
gf	-422.66	kJ/mol	Joback Method
hf	-949.18	kJ/mol	Joback Method
hfus	45.84	kJ/mol	Joback Method
hvap	90.92	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	1.549		Crippen Method
mcvol	277.320	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2553.00		NIST Webbook
tb	950.01	K	Joback Method
tc	1170.61	K	Joback Method
tf	594.33	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.19	J/mol×K	950.01	Joback Method
cpg	943.53	J/mol×K	986.78	Joback Method
cpg	955.33	J/mol×K	1023.54	Joback Method
cpg	965.56	J/mol×K	1060.31	Joback Method
cpg	974.26	J/mol×K	1097.08	Joback Method
cpg	981.42	J/mol×K	1133.84	Joback Method
cpg	987.05	J/mol×K	1170.61	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=R169645&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