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

Inchi: InChI=1S/C18H29NO4/c1-5-6-7-8-14-13(9-10-15(14)20)11-16(21)19-17(12(2)3)18(22)23
InchiKey: GDPPAUUXPQZOBY-BIVWUOKDSA-N
Formula: C18H29NO4
SMILES: CCC=CCC1C(=O)CCC1CC(=O)NC(C(=O)OC)C(C)C
Mol. weight [g/mol]: 323.43

Physical Properties

Property code	Value	Unit	Source
gf	-191.18	kJ/mol	Joback Method
hf	-709.66	kJ/mol	Joback Method
hfus	39.53	kJ/mol	Joback Method
hvap	81.38	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.642		Crippen Method
mcvol	269.880	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	873.28	K	Joback Method
tc	1086.95	K	Joback Method
tf	507.17	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.39	J/mol×K	873.28	Joback Method
cpg	904.91	J/mol×K	908.89	Joback Method
cpg	920.05	J/mol×K	944.50	Joback Method
cpg	933.85	J/mol×K	980.12	Joback Method
cpg	946.32	J/mol×K	1015.73	Joback Method
cpg	957.48	J/mol×K	1051.34	Joback Method
cpg	967.37	J/mol×K	1086.95	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=R169685&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