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

Inchi: InChI=1S/C16H25NO4/c1-4-5-6-7-13-12(8-9-14(13)18)10-15(19)17-11(2)16(20)21-3/h5-

InchiKey: KQVCDAGLJZTYOG-ZXRMRLFRSA-N

Formula: C16H25NO4

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

Mol. weight [g/mol]: 295.37

Physical Properties

Property code	Value	Unit	Source
gf	-205.58	kJ/mol	Joback Method
hf	-663.10	kJ/mol	Joback Method
hfus	37.88	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.006		Crippen Method
mcvol	241.700	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2144.00		NIST Webbook
tb	827.96	K	Joback Method
tc	1040.89	K	Joback Method
tf	499.63	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.19	J/mol×K	827.96	Joback Method
cpg	786.42	J/mol×K	863.45	Joback Method
cpg	801.39	J/mol×K	898.94	Joback Method
cpg	815.12	J/mol×K	934.43	Joback Method
cpg	827.61	J/mol×K	969.92	Joback Method
cpg	838.89	J/mol×K	1005.40	Joback Method
cpg	848.98	J/mol×K	1040.89	Joback Method

Sources

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=R169625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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