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

Inchi: InChI=1S/C19H31NO4/c1-5-7-8-9-15-14(10-11-16(15)21)12-17(22)20-18(13(3)6-2)19(23

InchiKey: YAGOAONRDWKQSK-UWDYBAJUSA-N

Formula: C19H31NO4

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

Mol. weight [g/mol]: 337.45

Physical Properties

Property code	Value	Unit	Source
gf	-182.76	kJ/mol	Joback Method
hf	-730.30	kJ/mol	Joback Method
hfus	42.12	kJ/mol	Joback Method
hvap	83.60	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.032		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	2344.00		NIST Webbook
tb	896.16	K	Joback Method
tc	1109.88	K	Joback Method
tf	518.44	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.27	J/mol×K	896.16	Joback Method
cpg	964.81	J/mol×K	931.78	Joback Method
cpg	979.93	J/mol×K	967.40	Joback Method
cpg	993.68	J/mol×K	1003.02	Joback Method
cpg	1006.06	J/mol×K	1038.64	Joback Method
cpg	1017.11	J/mol×K	1074.26	Joback Method
cpg	1026.85	J/mol×K	1109.88	Joback Method

Sources

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=R169650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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