Dehydrojasmonic acid, Ile conjugate, methyl ester

Inchi: InChI=1S/C19H29NO4/c1-5-7-8-9-15-14(10-11-16(15)21)12-17(22)20-18(13(3)6-2)19(23

InchiKey: MDFCXIXKDNKNPM-QQRPDSCRSA-N

Formula: C19H29NO4

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

Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
gf	-94.92	kJ/mol	Joback Method
hf	-604.87	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.808		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	892.84	K	Joback Method
tc	1108.22	K	Joback Method
tf	516.68	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.91	J/mol×K	892.84	Joback Method
cpg	936.05	J/mol×K	928.74	Joback Method
cpg	950.81	J/mol×K	964.63	Joback Method
cpg	964.24	J/mol×K	1000.53	Joback Method
cpg	976.36	J/mol×K	1036.42	Joback Method
cpg	987.21	J/mol×K	1072.32	Joback Method
cpg	996.81	J/mol×K	1108.22	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=R539183&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