bis-Homojasmonic acid, Ile conjugate, methyl ester

Inchi: InChI=1S/C20H33NO4/c1-5-7-8-9-10-11-15-16(12-13-17(15)22)19(23)21-18(14(3)6-2)20

InchiKey: QGYGIGLKPMEWPT-LHXQQAQFSA-N

Formula: C20H33NO4

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

Mol. weight [g/mol]: 351.48

Physical Properties

Property code	Value	Unit	Source
gf	-174.34	kJ/mol	Joback Method
hf	-750.94	kJ/mol	Joback Method
hfus	44.71	kJ/mol	Joback Method
hvap	85.83	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.422		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2587.00		NIST Webbook
tb	919.04	K	Joback Method
tc	1133.58	K	Joback Method
tf	529.71	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.74	J/mol×K	919.04	Joback Method
cpg	1025.30	J/mol×K	954.80	Joback Method
cpg	1040.41	J/mol×K	990.55	Joback Method
cpg	1054.08	J/mol×K	1026.31	Joback Method
cpg	1066.36	J/mol×K	1062.07	Joback Method
cpg	1077.27	J/mol×K	1097.83	Joback Method
cpg	1086.84	J/mol×K	1133.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R539158&Units=SI
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

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