Guaia-1(10),11-dien-9-one

Inchi: InChI=1S/C15H22O/c1-9(2)12-7-5-10(3)13-8-6-11(4)14(13)15(12)16/h9,12-13H,3,5-8H2,
InchiKey: UYGROYIOOPLGAS-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C1CCC(C(C)C)C(=O)C2=C(C)CCC12
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
hfus	17.75	kJ/mol	Joback Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.70	J/mol×K	648.82	Joback Method
cpg	562.88	J/mol×K	686.78	Joback Method
cpg	582.76	J/mol×K	724.73	Joback Method
cpg	601.38	J/mol×K	762.69	Joback Method
cpg	618.74	J/mol×K	800.65	Joback Method
cpg	634.87	J/mol×K	838.60	Joback Method
cpg	649.79	J/mol×K	876.56	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R73214&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices