Selina-3,11-dien-14-al

Inchi: InChI=1S/C15H22O/c1-11(2)12-6-8-15(3)7-4-5-13(10-16)14(15)9-12/h5,10,12,14H,1,4,6-
InchiKey: HAGXJRWOGHAEIY-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC2(C)CCC=C(C=O)C2C1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
hfus	17.78	kJ/mol	Joback Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
rinpol	1733.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.69	J/mol×K	618.09	Joback Method
cpg	548.77	J/mol×K	655.93	Joback Method
cpg	568.56	J/mol×K	693.77	Joback Method
cpg	587.20	J/mol×K	731.60	Joback Method
cpg	604.88	J/mol×K	769.44	Joback Method
cpg	621.77	J/mol×K	807.28	Joback Method
cpg	638.01	J/mol×K	845.12	Joback Method

Sources

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=R613088&Units=SI
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

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