Selina-3,11-dien-14-oic acid

Inchi: InChI=1S/C15H22O2/c1-10(2)11-6-8-15(3)7-4-5-12(14(16)17)13(15)9-11/h5,11,13H,1,4,
InchiKey: OKCQGVKXNGQQFZ-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C(C)C1CCC2(C)CCC=C(C(=O)O)C2C1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
hfus	21.18	kJ/mol	Joback Method
logp	3.790		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
rinpol	1777.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1777.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.65	J/mol×K	715.48	Joback Method
cpg	612.07	J/mol×K	751.25	Joback Method
cpg	628.67	J/mol×K	787.02	Joback Method
cpg	644.60	J/mol×K	822.80	Joback Method
cpg	659.99	J/mol×K	858.57	Joback Method
cpg	674.98	J/mol×K	894.34	Joback Method
cpg	689.73	J/mol×K	930.11	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=R613093&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