Selina-4,11-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/h11H,1,4-9H2,
InchiKey: UPRJMZGSOCQFML-NHYWBVRUSA-N
Formula: C15H22O2
SMILES: C=C(C)C1CCC2(C)CCCC(C(=O)O)=C2C1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
hfus	19.72	kJ/mol	Joback Method
logp	3.934		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.25	J/mol×K	725.13	Joback Method
cpg	608.13	J/mol×K	761.04	Joback Method
cpg	624.28	J/mol×K	796.95	Joback Method
cpg	639.83	J/mol×K	832.86	Joback Method
cpg	654.94	J/mol×K	868.78	Joback Method
cpg	669.74	J/mol×K	904.69	Joback Method
cpg	684.38	J/mol×K	940.60	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R73349&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

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