Selina-3,11-dien-9-ol

Inchi: InChI=1S/C15H24O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)14(16)9-12/h6,12-14,16H,1,5,7-

InchiKey: IVRQVIHZMLFDBK-URGYJCLVSA-N

Formula: C15H24O

SMILES: C=C(C)C1CC(O)C2(C)CCC=C(C)C2C1

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	20.65	kJ/mol	Joback Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.99	J/mol×K	656.94	Joback Method
cpg	593.37	J/mol×K	691.65	Joback Method
cpg	611.74	J/mol×K	726.36	Joback Method
cpg	629.25	J/mol×K	761.06	Joback Method
cpg	646.00	J/mol×K	795.77	Joback Method
cpg	662.12	J/mol×K	830.48	Joback Method
cpg	677.75	J/mol×K	865.19	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R73317&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