Selina-4,11-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/h10,12H,1,4-9H2,2-
InchiKey: VNYQZKHAWVXJCR-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC2(C)CCCC(C=O)=C2C1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
hfus	16.32	kJ/mol	Joback Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
rinpol	1765.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1758.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.25	J/mol×K	627.74	Joback Method
cpg	546.54	J/mol×K	665.73	Joback Method
cpg	565.61	J/mol×K	703.71	Joback Method
cpg	583.64	J/mol×K	741.70	Joback Method
cpg	600.80	J/mol×K	779.69	Joback Method
cpg	617.25	J/mol×K	817.67	Joback Method
cpg	633.16	J/mol×K	855.66	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R613122&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