

Selina-3,11-dien-9-one

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H22O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)14(16)9-12/h6,12-13H,1,5,7-9H

NCURUZQWQGIRTM-ILWWEHDPSA-N

C15H22O

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

218.33

Physical Properties

Property code	Value	Unit	Source
hfus	15.00	kJ/mol	Joback Method
hvap	68.61	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-4.16		Cheméo Relay (1.0)
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
tb	564.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.13	J/mol×K	637.25	Joback Method
cpg	562.46	J/mol×K	676.90	Joback Method
cpg	583.51	J/mol×K	716.54	Joback Method
cpg	603.42	J/mol×K	756.19	Joback Method
cpg	622.34	J/mol×K	795.83	Joback Method
cpg	640.42	J/mol×K	835.48	Joback Method
cpg	657.81	J/mol×K	875.13	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R73321&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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