

Selina-4(15),6-diene

Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h10-11,14H,3,5-9H2,1-2
InchiKey:	ALUIZDJKPCNAGJ-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1CCCC2(C)CCC(C(C)C)=CC12
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	12.33	kJ/mol	Joback Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1453.00		NIST Webbook
ripol	1618.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.60	J/mol×K	576.26	Joback Method
cpg	522.01	J/mol×K	613.40	Joback Method
cpg	543.03	J/mol×K	650.54	Joback Method
cpg	562.83	J/mol×K	687.68	Joback Method
cpg	581.54	J/mol×K	724.82	Joback Method
cpg	599.33	J/mol×K	761.96	Joback Method
cpg	616.34	J/mol×K	799.10	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R431277&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.cheméo.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
ripol:	Polar retention indices

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