

selin-4,7(11)-diene

Inchi: InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h5-10H2,1-4H3/t15-/m1/
InchiKey: CRIKCAXISSWYRQ-HNNXBMFYSA-N
Formula: C15H24
SMILES: CC(C)=C1CC[C@@]2(C)CCCC(C)=C2C1
Mol. weight [g/mol]: 204.36

Physical Properties

Property code	Value	Unit	Source
hfus	14.56	kJ/mol	Joback Method
logp	5.013		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1576.00		NIST Webbook
rinpol	1576.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1750.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.48	J/mol×K	593.71	Joback Method
cpg	522.03	J/mol×K	631.74	Joback Method
cpg	542.27	J/mol×K	669.77	Joback Method
cpg	561.37	J/mol×K	707.80	Joback Method
cpg	579.50	J/mol×K	745.83	Joback Method
cpg	596.84	J/mol×K	783.86	Joback Method
cpg	613.56	J/mol×K	821.89	Joback Method

Sources

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=R331776&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/ci990307I>

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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