

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-/m0/
InchiKey:	CRIKCAXISSWYRQ-HNNXBMFYSA-N
Formula:	C15H24
SMILES:	CC(C)=C1CCC2(C)CCCC(C)=C2C1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	198.35	kJ/mol	Joback Method
hf	-95.31	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.013		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpola	1576.00		NIST Webbook
ripola	1750.00		NIST Webbook
tb	593.71	K	Joback Method
tc	821.89	K	Joback Method
tf	330.95	K	Joback Method
vc	0.727	m ³ /kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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