Selina-3,7(11)-diene

Other names:	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(1-methylethylidene)-, (4aR-trans)- Eudesma-3,7(11)-diene 4a,8-Dimethyl-2-(1-methylethylidene)-1,2,3,4,4a,5,6,8a-octahydronaphthalene-, (4aR-trans)- 3,7(11)-Selinadiene Selina-3,7(11)-dien
Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h6,14H,5,7-10H2,1-4H3/
InchiKey:	WNRBYZQFEBIUGD-CABCVRRESA-N
Formula:	C15H24
SMILES:	CC1=CCCC2(C)CCC(=C(C)C)CC12
Mol. weight [g/mol]:	204.35
CAS:	6813-21-4

Physical Properties

Property code	Value	Unit	Source
gf	200.27	kJ/mol	Joback Method
hf	-104.18	kJ/mol	Joback Method
hfus	16.02	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1540.00		NIST Webbook

rinpol	1544.00	NIST Webbook
rinpol	1530.00	NIST Webbook
rinpol	1550.50	NIST Webbook
rinpol	1539.00	NIST Webbook
rinpol	1546.00	NIST Webbook
rinpol	1538.00	NIST Webbook
rinpol	1547.00	NIST Webbook
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ripol	1776.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1776.00		NIST Webbook
tb	584.06	K	Joback Method
tc	811.24	K	Joback Method
tf	314.19	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.06	J/mol×K	584.06	Joback Method
cpg	523.47	J/mol×K	621.92	Joback Method
cpg	544.48	J/mol×K	659.79	Joback Method
cpg	564.25	J/mol×K	697.65	Joback Method
cpg	582.97	J/mol×K	735.51	Joback Method
cpg	600.80	J/mol×K	773.38	Joback Method
cpg	617.92	J/mol×K	811.24	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6813214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume