

selina-3,7-diene

Inchi:

InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h6-7,11,14H,5,8-10H2,1

InchiKey:

SWCOCRTVQQHGKB-LOACHALJSA-N

Formula:

C15H24

SMILES:

CC1=CCCC2(C)CC=C(C(C)C)CC12

Mol. weight [g/mol]:

204.35

Physical Properties

Property code	Value	Unit	Source
gf	181.25	kJ/mol	Joback Method
hf	-129.39	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	49.87	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
ripol	1720.00		NIST Webbook
tb	581.24	K	Joback Method
tc	805.31	K	Joback Method
tf	316.07	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.03	J/mol×K	581.24	Joback Method
cpg	523.21	J/mol×K	618.59	Joback Method
cpg	544.03	J/mol×K	655.93	Joback Method
cpg	563.63	J/mol×K	693.28	Joback Method
cpg	582.18	J/mol×K	730.62	Joback Method
cpg	599.82	J/mol×K	767.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R234843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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