

Selin-7(11)-en-4-ol

Inchi:	InChI=1S/C15H26O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h13,16H,5-10H2,1-4H
InchiKey:	STRABSCAWZINIF-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC(C)=C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	29.92	kJ/mol	Joback Method
hf	-307.82	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.064		Crippen Method
mvol	202.060	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1696.00		NIST Webbook
tb	667.67	K	Joback Method
tc	882.48	K	Joback Method
tf	381.39	K	Joback Method
vc	0.755	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.41	J/mol×K	667.67	Joback Method
cpg	612.10	J/mol×K	703.47	Joback Method
cpg	630.99	J/mol×K	739.27	Joback Method
cpg	649.30	J/mol×K	775.07	Joback Method
cpg	667.26	J/mol×K	810.88	Joback Method
cpg	685.10	J/mol×K	846.68	Joback Method
cpg	703.04	J/mol×K	882.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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