

Selin-6-en-4«alpha»-ol

Inchi:	InChI=1S/C15H26O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h10-11,13,16H,5-9H
InchiKey:	PBGYWCDUYHJYFV-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC(C)C1=CC2C(C)(O)CCCC2(C)CC1
Mol. weight [g/mol]:	222.37
CAS:	118173-08-3

Physical Properties

Property code	Value	Unit	Source
gf	10.90	kJ/mol	Joback Method
hf	-333.03	kJ/mol	Joback Method
hfus	12.35	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1636.30		NIST Webbook
tb	664.85	K	Joback Method
tc	877.11	K	Joback Method
tf	383.27	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.44	J/mol×K	664.85	Joback Method
cpg	611.95	J/mol×K	700.23	Joback Method
cpg	630.65	J/mol×K	735.60	Joback Method
cpg	648.74	J/mol×K	770.98	Joback Method
cpg	666.45	J/mol×K	806.36	Joback Method
cpg	683.99	J/mol×K	841.73	Joback Method
cpg	701.57	J/mol×K	877.11	Joback Method

Sources

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=C118173083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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