

Selin-1-en-4-«alpha»-ol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H26O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h5,7,11-13,16H,6,8

GISHVTUWQQSNBW-AJNGGQMLSA-N

C15H26O

CC(C)C1CCC2(C)C=CCC(C)(O)C2C1

222.37

Physical Properties

Property code	Value	Unit	Source
gf	12.82	kJ/mol	Joback Method
hf	-341.90	kJ/mol	Joback Method
hfus	13.81	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
ripol	2273.00		NIST Webbook
tb	655.20	K	Joback Method
tc	866.56	K	Joback Method
tf	366.51	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.29	J/mol×K	655.20	Joback Method
cpg	614.43	J/mol×K	690.43	Joback Method
cpg	633.65	J/mol×K	725.65	Joback Method
cpg	652.18	J/mol×K	760.88	Joback Method
cpg	670.22	J/mol×K	796.11	Joback Method
cpg	687.97	J/mol×K	831.33	Joback Method
cpg	705.66	J/mol×K	866.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R560904&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

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

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