Selin-11-en-4-«alpha»-ol

Other names:	Kongol
	«alpha»-Selin-11-en-4-ol
	«alpha»-11-selinene-4-ol
	Selina-11-en-4-«alpha»-ol
	selin-11-en-4-«alpha»-ol (kongol)
	Eudesm-11-en-4a-ol
	11-Selinen-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/h12-13,16H,1,5-10H
InchiKey:	DPQYOKVMVCQHMY-AJNGGQMLSA-N
Formula:	C15H26O
SMILES:	C=C(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]:	222.37
CAS:	16641-47-7

Physical Properties

Property code	Value	Unit	Source
gf	64.59	kJ/mol	Joback Method
hf	-278.76	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1641.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1656.00		NIST Webbook
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rinpol	1653.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1635.00		NIST Webbook

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ripol	2282.00	NIST Webbook
ripol	2254.00	NIST Webbook
ripol	2239.00	NIST Webbook
ripol	2249.00	NIST Webbook

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ripol	2253.00		NIST Webbook
ripol	2216.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2263.00		NIST Webbook
tb	653.04	K	Joback Method
tc	865.92	K	Joback Method
tf	365.03	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.33	J/mol×K	653.04	Joback Method
cpg	613.82	J/mol×K	688.52	Joback Method
cpg	633.38	J/mol×K	724.00	Joback Method
cpg	652.21	J/mol×K	759.48	Joback Method
cpg	670.53	J/mol×K	794.96	Joback Method
cpg	688.57	J/mol×K	830.44	Joback Method
cpg	706.54	J/mol×K	865.92	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16641477&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
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