Selin-11-en-4-ol

Other names: 11-selinen-4-ol
Eudesm-11-en-4-ol
11-Selinene-4-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-MIGSVPMKSA-N
Formula: C15H26O
SMILES: C=C(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	13.52	kJ/mol	Joback Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1653.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1614.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2230.00		NIST Webbook
ripol	2230.00		NIST Webbook
ripol	2264.00		NIST Webbook

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R199047&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices