«alpha»-Caryophylladienol

Inchi: InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h12-14,16H,1-2,5-9
InchiKey: CIIYOYPOMGIECX-IHRRRGAJSA-N
Formula: C15H24O
SMILES: C=C1CCC2C(CC2(C)C)C(=C)CCC1O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	17.99	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Cheméo Relay (1.0)
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1661.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1634.00		NIST Webbook
ripol	2299.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2292.00		NIST Webbook
ripol	2299.00		NIST Webbook
tb	577.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.21	J/mol×K	658.83	Joback Method

cpg	594.89	J/mol×K	693.49	Joback Method
cpg	613.57	J/mol×K	728.16	Joback Method
cpg	631.35	J/mol×K	762.82	Joback Method
cpg	648.34	J/mol×K	797.48	Joback Method
cpg	664.64	J/mol×K	832.14	Joback Method
cpg	680.34	J/mol×K	866.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R325538&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

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