Cuprenenol

Inchi: InChI=1S/C15H26O/c1-12-6-10-15(16,11-7-12)14(4)9-5-8-13(14,2)3/h6,16H,5,7-11H2,1-
InchiKey: JXGLOXHHKFQUPA-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC1=CCC(O)(C2(C)CCCC2(C)C)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	7.47	kJ/mol	Joback Method
hvap	82.36	kJ/mol	Cheméo Relay (1.0)
logp	4.064		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1702.80		NIST Webbook
rinpol	1715.40		NIST Webbook
rinpol	1702.80		NIST Webbook
tb	551.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.96	J/mol×K	669.80	Joback Method
cpg	610.99	J/mol×K	706.85	Joback Method
cpg	630.41	J/mol×K	743.90	Joback Method
cpg	649.54	J/mol×K	780.95	Joback Method
cpg	668.73	J/mol×K	818.00	Joback Method
cpg	688.28	J/mol×K	855.05	Joback Method
cpg	708.53	J/mol×K	892.10	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=C943525664&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
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature