1,7-di-epi-«alpha»-Cedrenal

Inchi: InChI=1S/C15H22O/c1-10-4-5-13-14(2,3)12-8-15(10,13)7-6-11(12)9-16/h6,9-10,12-13H,
InchiKey: OETRFUZAVAFOBR-IKVITTDRSA-N
Formula: C15H22O
SMILES: CC1CCC2C(C)(C)C3CC12CC=C3C=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
hfus	17.48	kJ/mol	Joback Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tf	339.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.87	J/mol×K	615.30	Joback Method
cpg	551.35	J/mol×K	653.25	Joback Method
cpg	570.61	J/mol×K	691.20	Joback Method
cpg	588.97	J/mol×K	729.15	Joback Method
cpg	606.73	J/mol×K	767.10	Joback Method
cpg	624.18	J/mol×K	805.04	Joback Method
cpg	641.63	J/mol×K	842.99	Joback Method

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R625546&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tf:	Normal melting (fusion) point