5-Isocedranol

Inchi: InChI=1S/C15H26O/c1-10-5-7-14-9-12(10)13(3,4)15(14,16)8-6-11(14)2/h10-12,16H,5-9H
InchiKey: NDWXPZSIXZULJI-ZGVRZNAHSA-N
Formula: C15H26O
SMILES: CC1CCC23CC1C(C)(C)C2(O)CCC3C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	13.22	kJ/mol	Joback Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
rinpol	1676.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/mol×K	650.25	Joback Method
cpg	615.74	J/mol×K	685.82	Joback Method
cpg	634.97	J/mol×K	721.39	Joback Method
cpg	653.76	J/mol×K	756.96	Joback Method
cpg	672.45	J/mol×K	792.52	Joback Method
cpg	691.37	J/mol×K	828.09	Joback Method
cpg	710.84	J/mol×K	863.66	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R625219&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):	

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