(-)-«alpha»-helmiscapene

Other names: «alpha»-helmiscapene
Inchi: InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h6,13-14H,1,5,7-10H2,2-
InchiKey: OZQAPQSEYFAMCY-LOWNFYCTSA-N
Formula: C15H24
SMILES: C=C(C)C1CCC2(C)CCC=C(C)C2C1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	15.49	kJ/mol	Joback Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/mol×K	569.43	Joback Method
cpg	523.17	J/mol×K	606.91	Joback Method
cpg	545.19	J/mol×K	644.39	Joback Method
cpg	565.88	J/mol×K	681.87	Joback Method
cpg	585.40	J/mol×K	719.35	Joback Method
cpg	603.90	J/mol×K	756.83	Joback Method
cpg	621.57	J/mol×K	794.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R141870&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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices