Dihydrochamazulene 4

Inchi: InChI=1S/C15H20/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h6,8-10H,5,7H2,1-4H3
InchiKey: HHROSHNZYCROCO-UHFFFAOYSA-N
Formula: C15H20
SMILES: CC1=C2C=C(C(C)C)CCC(C)=C2C=C1
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	233.19	kJ/mol	Joback Method
hf	-22.80	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.565		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	603.60	K	Joback Method
tc	826.16	K	Joback Method
tf	339.73	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.02	J/mol×K	603.60	Joback Method
cpg	478.25	J/mol×K	640.69	Joback Method
cpg	495.37	J/mol×K	677.79	Joback Method
cpg	511.45	J/mol×K	714.88	Joback Method
cpg	526.54	J/mol×K	751.98	Joback Method
cpg	540.71	J/mol×K	789.07	Joback Method
cpg	554.02	J/mol×K	826.16	Joback Method
dvisc	0.0015052	Pa×s	339.73	Joback Method

dvisc	0.0009265	Pa×s	383.71	Joback Method
dvisc	0.0006301	Pa×s	427.69	Joback Method
dvisc	0.0004605	Pa×s	471.67	Joback Method
dvisc	0.0003550	Pa×s	515.64	Joback Method
dvisc	0.0002851	Pa×s	559.62	Joback Method
dvisc	0.0002364	Pa×s	603.60	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R633691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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