Dihydrochamazulene 1

Inchi: InChI=1S/C15H20/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h5-10,12,15H,1-4H3
InchiKey: PFKPSYLPTIZOLX-UHFFFAOYSA-N
Formula: C15H20
SMILES: CC1=C2C=CC(C)C2C=C(C(C)C)C=C1
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	237.03	kJ/mol	Joback Method
hf	-40.54	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.277		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tb	584.30	K	Joback Method
tc	804.86	K	Joback Method
tf	306.21	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.66	J/mol×K	584.30	Joback Method
cpg	482.45	J/mol×K	621.06	Joback Method
cpg	501.03	J/mol×K	657.82	Joback Method
cpg	518.45	J/mol×K	694.58	Joback Method
cpg	534.78	J/mol×K	731.34	Joback Method
cpg	550.06	J/mol×K	768.10	Joback Method
cpg	564.36	J/mol×K	804.86	Joback Method
dvisc	0.0015832	Pa×s	306.21	Joback Method

dvisc	0.0010106	Pa×s	352.56	Joback Method
dvisc	0.0007160	Pa×s	398.91	Joback Method
dvisc	0.0005450	Pa×s	445.25	Joback Method
dvisc	0.0004368	Pa×s	491.60	Joback Method
dvisc	0.0003637	Pa×s	537.95	Joback Method
dvisc	0.0003117	Pa×s	584.30	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=R633666&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