3,6-Dihydrochamazulene

Inchi: InChI=1S/C14H18/c1-4-12-7-5-10(2)13-8-6-11(3)14(13)9-12/h5-6,9H,4,7-8H2,1-3H3
InchiKey: NVMJWYJTLVURAS-UHFFFAOYSA-N
Formula: C14H18
SMILES: CCC1=CC2=C(CC=C2C)C(C)=CC1
Mol. weight [g/mol]: 186.29
CAS: 18454-88-1

Physical Properties

Property code	Value	Unit	Source
gf	227.21	kJ/mol	Joback Method
hf	3.12	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.319		Crippen Method
mcvol	169.200	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1518.70		NIST Webbook
rinpol	1518.70		NIST Webbook
ripol	2350.00		NIST Webbook
tb	581.16	K	Joback Method
tc	803.09	K	Joback Method
tf	343.46	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.59	J/mol×K	581.16	Joback Method
cpg	426.83	J/mol×K	618.15	Joback Method
cpg	443.03	J/mol×K	655.14	Joback Method
cpg	458.26	J/mol×K	692.12	Joback Method
cpg	472.56	J/mol×K	729.11	Joback Method
cpg	486.00	J/mol×K	766.10	Joback Method

cpg	498.62	J/mol×K	803.09	Joback Method
dvisc	0.0012701	Pa×s	343.46	Joback Method
dvisc	0.0008570	Pa×s	383.08	Joback Method
dvisc	0.0006225	Pa×s	422.69	Joback Method
dvisc	0.0004777	Pa×s	462.31	Joback Method
dvisc	0.0003822	Pa×s	501.93	Joback Method
dvisc	0.0003159	Pa×s	541.54	Joback Method
dvisc	0.0002680	Pa×s	581.16	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C18454881&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume