

Dehydrochamazulene

Inchi:	InChI=1S/C14H14/c1-4-12-7-5-10(2)13-8-6-11(3)14(13)9-12/h4-9H,1H2,2-3H3
InchiKey:	RDXQLYFNEFLBQI-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	<chem>C=Cc1ccc(C)c2ccc(C)c-2c1</chem>
Mol. weight [g/mol]:	182.26
CAS:	321732-25-6

Physical Properties

Property code	Value	Unit	Source
gf	345.01	kJ/mol	Joback Method
hf	186.33	kJ/mol	Joback Method
hfus	20.63	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.051		Crippen Method
mvol	160.600	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1784.60		NIST Webbook
tb	577.00	K	Joback Method
tc	805.94	K	Joback Method
tf	342.46	K	Joback Method
vc	0.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.27	J/molxK	577.00	Joback Method
cpg	384.67	J/molxK	615.16	Joback Method
cpg	399.06	J/molxK	653.31	Joback Method
cpg	412.49	J/molxK	691.47	Joback Method
cpg	425.05	J/molxK	729.62	Joback Method
cpg	436.79	J/molxK	767.78	Joback Method
cpg	447.78	J/molxK	805.94	Joback Method
dvisc	0.0010914	Paxs	342.46	Joback Method

dvisc	0.0007747	Paxs	381.55	Joback Method
dvisc	0.0005861	Paxs	420.64	Joback Method
dvisc	0.0004649	Paxs	459.73	Joback Method
dvisc	0.0003824	Paxs	498.82	Joback Method
dvisc	0.0003237	Paxs	537.91	Joback Method
dvisc	0.0002802	Paxs	577.00	Joback Method

Sources

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=C321732256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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