Chamazulene

Other names:	Azulene, 7-ethyl-1,4-dimethyl- Ba 2784 Camazulene Chamazulen Dimethulene 1,4-Dimethyl-7-ethylazulene 7-Ethyl-1,4-dimethylazulene Azulene, 1,4-dimethyl-7-ethyl- Dimethulen
Inchi:	InChI=1S/C14H16/c1-4-12-7-5-10(2)13-8-6-11(3)14(13)9-12/h5-9H,4H2,1-3H3
InchiKey:	GXGJIOMUZAGVEH-UHFFFAOYSA-N
Formula:	C14H16
SMILES:	CCc1ccc(C)c2ccc(C)c-2c1
Mol. weight [g/mol]:	184.28
CAS:	529-05-5

Physical Properties

Property code	Value	Unit	Source
gf	257.17	kJ/mol	Joback Method
hf	60.90	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	52.66	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.971		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1732.00		NIST Webbook

rinpol	1707.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1725.00		NIST Webbook
ripol	2380.00		NIST Webbook
ripol	2396.00		NIST Webbook
ripol	2360.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2370.00		NIST Webbook
tb	580.32	K	Joback Method
tc	804.38	K	Joback Method
tf	344.22	K	Joback Method

vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.57	J/mol×K	580.32	Joback Method
cpg	460.53	J/mol×K	767.04	Joback Method
cpg	448.10	J/mol×K	729.69	Joback Method
cpg	434.85	J/mol×K	692.35	Joback Method
cpg	420.71	J/mol×K	655.01	Joback Method
cpg	405.64	J/mol×K	617.66	Joback Method
cpg	472.20	J/mol×K	804.38	Joback Method
dvisc	0.0002732	Pa×s	580.32	Joback Method
dvisc	0.0003180	Pa×s	540.97	Joback Method
dvisc	0.0003791	Pa×s	501.62	Joback Method
dvisc	0.0004655	Pa×s	462.27	Joback Method
dvisc	0.0005940	Pa×s	422.92	Joback Method
dvisc	0.0007967	Pa×s	383.57	Joback Method
dvisc	0.0011430	Pa×s	344.22	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C529055&Units=SI
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

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