

cis-Chrysanthenol

Other names:	Chrysanthenol (Z)-chrysanthenol
Inchi:	InChI=1S/C10H16O/c1-6-4-5-7-9(11)8(6)10(7,2)3/h4,7-9,11H,5H2,1-3H3
InchiKey:	IRZWAJHUWGZMMT-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CCC2C(O)C1C2(C)C
Mol. weight [g/mol]:	152.23
CAS:	55722-60-6

Physical Properties

Property code	Value	Unit	Source
gf	5.32	kJ/mol	Joback Method
hf	-241.65	kJ/mol	Joback Method
hfus	16.59	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1146.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1162.00		NIST Webbook
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rinpol	1163.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1161.00		NIST Webbook
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rinpol	1162.00		NIST Webbook
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rinpol	1165.00		NIST Webbook
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rinpol	1155.00		NIST Webbook
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rinpol	1147.00		NIST Webbook
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rinpol	1162.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1173.50		NIST Webbook
rinpol	1143.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1716.00		NIST Webbook
tb	533.17	K	Joback Method
tc	729.30	K	Joback Method
tf	324.34	K	Joback Method
vc	0.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	336.85	J/mol×K	533.17	Joback Method
cpg	351.53	J/mol×K	565.86	Joback Method
cpg	365.30	J/mol×K	598.55	Joback Method
cpg	378.26	J/mol×K	631.23	Joback Method
cpg	390.53	J/mol×K	663.92	Joback Method
cpg	402.21	J/mol×K	696.61	Joback Method
cpg	413.40	J/mol×K	729.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C55722606&Units=SI

Legend

cpg:	Ideal gas heat capacity
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

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