

Bicyclo[3.1.1]hept-2-en-6-one, 2,7,7-trimethyl-

Other names:	Chrysanthenone 2-Pinen-7-one Isochrysanthenone Chrysantenone Crysanthenone
Inchi:	InChI=1S/C10H14O/c1-6-4-5-7-9(11)8(6)10(7,2)3/h4,7-8H,5H2,1-3H3
InchiKey:	IECBDTGWSQNQID-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC1=CCC2C(=O)C1C2(C)C
Mol. weight [g/mol]:	150.22
CAS:	473-06-3

Physical Properties

Property code	Value	Unit	Source
gf	27.26	kJ/mol	Joback Method
hf	-206.78	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	41.59	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1121.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook

rinpol	1124.00	NIST Webbook
rinpol	1123.00	NIST Webbook
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rinpol	1131.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1103.00	NIST Webbook
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rinpol	1121.00	NIST Webbook
rinpol	1094.00	NIST Webbook
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rinpol	1126.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1123.00	NIST Webbook
rinpol	1100.00	NIST Webbook
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rinpol	1102.00	NIST Webbook
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rinpol	1096.00		NIST Webbook
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rinpol	1106.00		NIST Webbook
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ripol	1501.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1500.00		NIST Webbook
tb	513.48	K	Joback Method
tc	740.08	K	Joback Method
tf	335.98	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.39	J/mol×K	513.48	Joback Method
cpg	324.08	J/mol×K	551.25	Joback Method
cpg	339.67	J/mol×K	589.01	Joback Method
cpg	354.29	J/mol×K	626.78	Joback Method
cpg	368.08	J/mol×K	664.55	Joback Method
cpg	381.17	J/mol×K	702.31	Joback Method
cpg	393.70	J/mol×K	740.08	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=C473063&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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