

Santolina triene

Inchi:	InChI=1S/C10H16/c1-6-10(9(4)5)7-8(2)3/h6-7,10H,1,4H2,2-3,5H3
InchiKey:	ZQGDEJAPCUGBRH-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	<chem>C=CC(C=C(C)C)C(=C)C</chem>
Mol. weight [g/mol]:	136.23
CAS:	2153-66-4

Physical Properties

Property code	Value	Unit	Source
gf	269.68	kJ/mol	Joback Method
hf	93.49	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	36.24	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.331		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	900.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	902.00		NIST Webbook
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rinpol	909.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	901.00		NIST Webbook
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rinpol	906.90		NIST Webbook
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rinpol	900.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	901.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1024.00		NIST Webbook
ripol	1027.00		NIST Webbook
ripol	1018.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1011.00		NIST Webbook
ripol	1063.00		NIST Webbook
tb	425.04	K	Joback Method
tc	613.42	K	Joback Method
tf	150.94	K	Joback Method
vc	0.533	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.95	J/mol×K	425.04	Joback Method
cpg	282.78	J/mol×K	456.44	Joback Method
cpg	296.84	J/mol×K	487.83	Joback Method
cpg	310.16	J/mol×K	519.23	Joback Method
cpg	322.78	J/mol×K	550.63	Joback Method
cpg	334.72	J/mol×K	582.02	Joback Method
cpg	346.04	J/mol×K	613.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2153664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
ripol:	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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