

Santolina alcohol

Inchi: InChI=1S/C10H18O/c1-6-9(7-8(2)3)10(4,5)11/h6-7,9,11H,1H2,2-5H3
InchiKey: JWGLVEFPXSKNBN-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C=CC(C=C(C)C)C(C)(C)O
Mol. weight [g/mol]: 154.25
CAS: 21149-19-9

Physical Properties

Property code	Value	Unit	Source
gf	56.41	kJ/mol	Joback Method
hf	-183.13	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	52.22	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.526		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1030.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1051.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1375.00		NIST Webbook

tb	517.43	K	Joback Method
tc	700.79	K	Joback Method
tf	229.90	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.28	J/mol×K	517.43	Joback Method
cpg	360.97	J/mol×K	547.99	Joback Method
cpg	373.89	J/mol×K	578.55	Joback Method
cpg	386.07	J/mol×K	609.11	Joback Method
cpg	397.57	J/mol×K	639.67	Joback Method
cpg	408.42	J/mol×K	670.23	Joback Method
cpg	418.68	J/mol×K	700.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21149199&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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