cis-Tagetenone

Inchi: InChI=1S/C10H14O/c1-5-9(4)7-10(11)6-8(2)3/h5-7H,1H2,2-4H3/b9-7-
InchiKey: XUINKEIPBTYUJP-CLFYSBASSA-N
Formula: C10H14O
SMILES: C=CC(C)=CC(=O)C=C(C)C
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	135.58	kJ/mol	Joback Method
hf	-22.02	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.654		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1232.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
tb	486.83	K	Joback Method
tc	686.94	K	Joback Method
tf	212.55	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.46	J/mol×K	486.83	Joback Method
cpg	304.04	J/mol×K	520.18	Joback Method
cpg	316.83	J/mol×K	553.53	Joback Method
cpg	328.85	J/mol×K	586.88	Joback Method
cpg	340.17	J/mol×K	620.23	Joback Method

cpg	350.82	J/mol×K	653.59	Joback Method
cpg	360.87	J/mol×K	686.94	Joback Method

Sources

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=R628738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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