

(Z)-Tagetone

Inchi:	InChI=1S/C10H16O/c1-5-9(4)7-10(11)6-8(2)3/h5,7-8H,1,6H2,2-4H3/b9-7-
InchiKey:	RJXKHBTYHGBOKV-CLFYSBASSA-N
Formula:	C10H16O
SMILES:	<chem>C=CC(C)=CC(=O)CC(C)C</chem>
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	61.47	kJ/mol	Joback Method
hf	-134.73	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1152.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1123.00		NIST Webbook
tb	482.35	K	Joback Method
tc	674.03	K	Joback Method
tf	216.59	K	Joback Method
vc	0.557	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.71	J/molxK	482.35	Joback Method
cpg	321.86	J/molxK	514.30	Joback Method
cpg	335.28	J/molxK	546.24	Joback Method
cpg	347.99	J/molxK	578.19	Joback Method
cpg	360.04	J/molxK	610.14	Joback Method
cpg	371.44	J/molxK	642.09	Joback Method
cpg	382.25	J/molxK	674.03	Joback Method

Sources

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=R607182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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