

Tagetonol

Inchi:	InChI=1S/C10H18O2/c1-5-10(4,12)7-9(11)6-8(2)3/h5,8,12H,1,6-7H2,2-4H3
InchiKey:	HPKAJXIDKBSLHJ-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	<chem>C=CC(C)(O)CC(=O)CC(C)C</chem>
Mol. weight [g/mol]:	170.25
CAS:	71547-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-144.18	kJ/mol	Joback Method
hf	-403.14	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	58.92	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.929		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1136.00		NIST Webbook
tb	567.26	K	Joback Method
tc	748.60	K	Joback Method
tf	298.87	K	Joback Method
vc	0.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.34	J/molxK	567.26	Joback Method
cpg	399.11	J/molxK	597.48	Joback Method
cpg	411.19	J/molxK	627.71	Joback Method
cpg	422.61	J/molxK	657.93	Joback Method
cpg	433.42	J/molxK	688.16	Joback Method
cpg	443.63	J/molxK	718.38	Joback Method
cpg	453.29	J/molxK	748.60	Joback Method
dvisc	0.0216284	Paxs	298.87	Joback Method

dvisc	0.0048525	Paxs	343.60	Joback Method
dvisc	0.0015362	Paxs	388.33	Joback Method
dvisc	0.0006167	Paxs	433.06	Joback Method
dvisc	0.0002937	Paxs	477.80	Joback Method
dvisc	0.0001589	Paxs	522.53	Joback Method
dvisc	0.0000947	Paxs	567.26	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=C71547632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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