

Tumerone

Inchi:	InChI=1S/C15H22O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5,7,9,13H,6,8,10H2,1
InchiKey:	ZMIQNSSHYBJKIL-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CC(C)=CC(=O)CC(C)C1=CC=C(C)CC1
Mol. weight [g/mol]:	218.33
CAS:	180315-67-7

Physical Properties

Property code	Value	Unit	Source
gf	88.55	kJ/mol	Joback Method
hf	-196.08	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	58.03	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1680.30		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1649.00		NIST Webbook
ripol	2245.00		NIST Webbook
ripol	2245.00		NIST Webbook
tb	632.57	K	Joback Method
tc	846.21	K	Joback Method
tf	312.88	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.50	J/mol×K	632.57	Joback Method
cpg	537.67	J/mol×K	668.18	Joback Method
cpg	554.74	J/mol×K	703.78	Joback Method
cpg	570.77	J/mol×K	739.39	Joback Method
cpg	585.82	J/mol×K	775.00	Joback Method
cpg	599.93	J/mol×K	810.60	Joback Method
cpg	613.17	J/mol×K	846.21	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=C180315677&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
mccvol:	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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