Ar-Turmerone

Other names:	Turmerone
	ar-tumerone
	Turmerone (-ar)
	Aromatic turmerone
Inchi:	InChI=1S/C15H20O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5-9,13H,10H2,1-4H3
InchiKey:	NAAJVHHFAXWBOK-UHFFFAOYSA-N
Formula:	C15H20O
SMILES:	CC(C)=CC(=O)CC(C)c1ccc(C)cc1
Mol. weight [g/mol]:	216.32
CAS:	532-65-0

Physical Properties

Property code	Value	Unit	Source
gf	118.51	kJ/mol	Joback Method
hf	-138.30	kJ/mol	Joback Method
hfus	25.23	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.024		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1672.30		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1637.00		NIST Webbook

rinpol	1662.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	631.73	K	Joback Method
tc	847.25	K	Joback Method
tf	313.64	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.60	J/mol×K	631.73	Joback Method
cpg	514.72	J/mol×K	667.65	Joback Method
cpg	530.78	J/mol×K	703.57	Joback Method
cpg	545.84	J/mol×K	739.49	Joback Method
cpg	559.95	J/mol×K	775.41	Joback Method
cpg	573.17	J/mol×K	811.33	Joback Method
cpg	585.56	J/mol×K	847.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C532650&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume