

ar-Turmerone

Other names:	Aromatic turmerone Turmerone Turmerone (-ar) ar-tumerone
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

Physical Properties

Property code	Value	Unit	Source
hfus	25.23	kJ/mol	Joback Method
ie	8.23	eV	Cheméo Relay (1.0)
logp	4.024		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
rinpol	1669.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1640.00		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	1638.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1659.00		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	1664.00		NIST Webbook
tb	540.45	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C532650&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

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