Turmerone (dihydro-ar)

Other names: Dihydro-Ar-turmerone
Inchi: InChI=1S/C15H22O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5-8,11,13H,9-10H2,1-
InchiKey: FWSUEHMNQCROMJ-UHFFFAOYSA-N
Formula: C15H22O
SMILES: Cc1ccc(C(C)CC(=O)CC(C)C)cc1
Mol. weight [g/mol]: 218.33
CAS: 4179-20-8

Physical Properties

Property code	Value	Unit	Source
gf	44.40	kJ/mol	Joback Method
hf	-251.01	kJ/mol	Joback Method
hfus	22.81	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.104		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
tb	627.25	K	Joback Method
tc	834.98	K	Joback Method
tf	317.68	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.15	J/mol×K	627.25	Joback Method
cpg	536.87	J/mol×K	661.87	Joback Method
cpg	553.56	J/mol×K	696.49	Joback Method
cpg	569.26	J/mol×K	731.11	Joback Method

cpg	584.00	J/mol×K	765.73	Joback Method
cpg	597.83	J/mol×K	800.36	Joback Method
cpg	610.78	J/mol×K	834.98	Joback Method
dvisc	0.0034484	Pa×s	317.68	Joback Method
dvisc	0.0014141	Pa×s	369.27	Joback Method
dvisc	0.0007215	Pa×s	420.87	Joback Method
dvisc	0.0004264	Pa×s	472.47	Joback Method
dvisc	0.0002795	Pa×s	524.06	Joback Method
dvisc	0.0001976	Pa×s	575.65	Joback Method
dvisc	0.0001479	Pa×s	627.25	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4179208&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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