

(.+/-)-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:	<chem>Cc1ccc(C(C)CC(=O)CC(C)C)cc1</chem>
Mol. weight [g/mol]:	218.33
CAS:	30666-87-6

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	1597.50		NIST Webbook
tb	627.25	K	Joback Method
tc	834.98	K	Joback Method
tf	317.68	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.15	J/molxK	627.25	Joback Method
cpg	536.87	J/molxK	661.87	Joback Method
cpg	553.56	J/molxK	696.49	Joback Method
cpg	569.26	J/molxK	731.11	Joback Method
cpg	584.00	J/molxK	765.73	Joback Method
cpg	597.83	J/molxK	800.36	Joback Method
cpg	610.78	J/molxK	834.98	Joback Method
dvisc	0.0034484	Paxs	317.68	Joback Method

dvisc	0.0014141	Paxs	369.27	Joback Method
dvisc	0.0007215	Paxs	420.87	Joback Method
dvisc	0.0004264	Paxs	472.47	Joback Method
dvisc	0.0002795	Paxs	524.06	Joback Method
dvisc	0.0001976	Paxs	575.65	Joback Method
dvisc	0.0001479	Paxs	627.25	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=C30666876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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