2-Methyl-6-(4-methylcyclohexa-2,4-dien-1-yl)hept-

Other names: «alpha»-Turmerone
Inchi: InChI=1S/C15H22O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5-7,9,13-14H,8,10H2,
InchiKey: XOCANRBEOZQNAQ-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC(C)=CC(=O)CC(C)C1C=CC(C)=CC1
Mol. weight [g/mol]: 218.33
CAS: 82508-15-4

Physical Properties

Property code	Value	Unit	Source
gf	90.47	kJ/mol	Joback Method
hf	-204.95	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.070		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1879.80		NIST Webbook
rinpol	1879.80		NIST Webbook
tb	622.92	K	Joback Method
tc	835.61	K	Joback Method
tf	296.12	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.27	J/mol×K	622.92	Joback Method
cpg	540.16	J/mol×K	658.37	Joback Method
cpg	557.90	J/mol×K	693.82	Joback Method
cpg	574.55	J/mol×K	729.27	Joback Method
cpg	590.16	J/mol×K	764.72	Joback Method
cpg	604.79	J/mol×K	800.16	Joback Method

cpg	618.48	J/mol×K	835.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82508154&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

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