

Curlone

Other names:	2-Hepten-4-one,2-methyl-6-[(1S)-4-methylene- 2-cyclohexen-1-yl]-, (6S)-«beta»-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,3,6,8,10
InchiKey:	JIJQKFPGBBEJNF-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	<chem>C=C1C=CC(C(C)CC(=O)C=C(C)C)CC1</chem>
Mol. weight [g/mol]:	218.33
CAS:	87440-60-6

Physical Properties

Property code	Value	Unit	Source
gf	123.22	kJ/mol	Joback Method
hf	-167.02	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.070		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1655.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	617.94	K	Joback Method
tc	829.53	K	Joback Method
tf	296.52	K	Joback Method
vc	0.759	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.32	J/mol×K	617.94	Joback Method
cpg	539.42	J/mol×K	653.20	Joback Method
cpg	557.36	J/mol×K	688.47	Joback Method
cpg	574.21	J/mol×K	723.73	Joback Method
cpg	590.00	J/mol×K	759.00	Joback Method
cpg	604.79	J/mol×K	794.26	Joback Method
cpg	618.63	J/mol×K	829.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C87440606&Units=SI

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

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