

trans-Humul-9(E)-en-2,6-dione

Inchi:	InChI=1S/C15H24O2/c1-11-6-5-9-15(3,4)10-14(17)12(2)7-8-13(11)16/h5,9,11-12H,6-8,1
InchiKey:	MSVVNYKZJZHJV-YRPDJFBCSA-N
Formula:	C15H24O2
SMILES:	CC1CC=CC(C)(C)CC(=O)C(C)CCC1=O
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	-196.76	kJ/mol	Joback Method
hf	-572.47	kJ/mol	Joback Method
hfus	12.03	kJ/mol	Joback Method
hvap	57.29	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.553		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1739.00		NIST Webbook
rinpol	1739.00		NIST Webbook
tb	709.20	K	Joback Method
tc	963.61	K	Joback Method
tf	401.21	K	Joback Method
vc	0.764	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.51	J/mol×K	709.20	Joback Method
cpg	657.10	J/mol×K	751.60	Joback Method
cpg	681.05	J/mol×K	794.00	Joback Method
cpg	703.38	J/mol×K	836.41	Joback Method
cpg	724.11	J/mol×K	878.81	Joback Method
cpg	743.27	J/mol×K	921.21	Joback Method
cpg	760.88	J/mol×K	963.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R421275&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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