Humulene-6,7-oxide

Inchi: InChI=1S/C15H22O/c1-11-6-5-8-15(3,4)9-7-12(2)14-13(10-11)16-14/h5,7-8,10,13-14H,6
InchiKey: CURDSHVMYFYNIX-GQRUBBQQSA-N
Formula: C15H22O
SMILES: CC1=CC2OC2C(C)=CCC(C)(C)C=CC1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	95.62	kJ/mol	Joback Method
hf	-230.99	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	55.09	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.023		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
ripol	2041.00		NIST Webbook
tb	611.66	K	Joback Method
tc	846.02	K	Joback Method
tf	347.12	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.59	J/mol×K	611.66	Joback Method
cpg	541.74	J/mol×K	650.72	Joback Method
cpg	562.54	J/mol×K	689.78	Joback Method
cpg	582.13	J/mol×K	728.84	Joback Method
cpg	600.66	J/mol×K	767.90	Joback Method
cpg	618.27	J/mol×K	806.96	Joback Method
cpg	635.11	J/mol×K	846.02	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=R439964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume