3-Isothujone

Inchi: InChI=1S/C10H16O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-8H,4-5H2,1-3H3/t7-,8-,10+/m1/s1
InchiKey: USMNOWBWPHYOEA-MRTMQBJTSA-N
Formula: C10H16O
SMILES: CC1C(=O)CC2(C(C)C)CC12
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	16.59	kJ/mol	Joback Method
hf	-252.21	kJ/mol	Joback Method
hfus	8.69	kJ/mol	Joback Method
hvap	40.08	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1103.00		NIST Webbook
ripol	1440.00		NIST Webbook
tb	504.63	K	Joback Method
tc	724.49	K	Joback Method
tf	311.22	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.27	J/mol×K	504.63	Joback Method
cpg	342.10	J/mol×K	541.27	Joback Method
cpg	358.73	J/mol×K	577.92	Joback Method
cpg	374.30	J/mol×K	614.56	Joback Method
cpg	388.94	J/mol×K	651.20	Joback Method
cpg	402.80	J/mol×K	687.84	Joback Method
cpg	416.01	J/mol×K	724.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409319&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume