3-Isothujyl acetate

Inchi: InChI=1S/C12H20O2/c1-7(2)12-5-10(12)8(3)11(6-12)14-9(4)13/h7-8,10-11H,5-6H2,1-4H
InchiKey: RYMWIDNPMDLHRP-RVHAWEMESA-N
Formula: C12H20O2
SMILES: CC(=O)OC1CC2(C(C)C)CC2C1C
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-85.61	kJ/mol	Joback Method
hf	-420.93	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.620		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1285.00		NIST Webbook
tb	554.19	K	Joback Method
tc	758.84	K	Joback Method
tf	333.46	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.10	J/mol×K	554.19	Joback Method
cpg	456.42	J/mol×K	588.30	Joback Method
cpg	473.65	J/mol×K	622.41	Joback Method
cpg	489.90	J/mol×K	656.52	Joback Method
cpg	505.31	J/mol×K	690.62	Joback Method
cpg	519.99	J/mol×K	724.73	Joback Method
cpg	534.06	J/mol×K	758.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R560677&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