Hushinone

Inchi: InChI=1S/C14H22O/c1-13(2)7-10-9-4-5-14(3,8-11(10)13)12(15)6-9/h9-11H,4-8H2,1-3H3
InchiKey: XLTFJFLEBDDNKD-RMIALFOJSA-N
Formula: C14H22O
SMILES: CC12CCC(CC1=O)C1CC(C)(C)C1C2
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	76.06	kJ/mol	Joback Method
hf	-274.11	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	48.17	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.428		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
ripol	2209.00		NIST Webbook
ripol	2209.00		NIST Webbook
ripol	2209.00		NIST Webbook
tb	607.44	K	Joback Method
tc	847.85	K	Joback Method
tf	401.86	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.23	J/mol×K	607.44	Joback Method
cpg	534.02	J/mol×K	647.51	Joback Method
cpg	555.46	J/mol×K	687.58	Joback Method
cpg	575.85	J/mol×K	727.65	Joback Method
cpg	595.52	J/mol×K	767.72	Joback Method
cpg	614.78	J/mol×K	807.79	Joback Method
cpg	633.95	J/mol×K	847.85	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=R340646&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume