

«gamma»-coronal

Inchi:	InChI=1S/C14H22O/c1-11(10-15)7-8-13-12(2)6-5-9-14(13,3)4/h10,13H,1-2,5-9H2,3-4H3
InchiKey:	WOGYNENARNGEFU-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	<chem>C=C(C=O)CCC1C(=C)CCCC1(C)C</chem>
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	111.10	kJ/mol	Joback Method
hf	-168.77	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	52.02	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
ripol	1888.00		NIST Webbook
ripol	1888.00		NIST Webbook
tb	579.22	K	Joback Method
tc	786.58	K	Joback Method
tf	314.54	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.33	J/mol×K	579.22	Joback Method
cpg	505.41	J/mol×K	613.78	Joback Method
cpg	523.43	J/mol×K	648.34	Joback Method
cpg	540.49	J/mol×K	682.90	Joback Method
cpg	556.71	J/mol×K	717.46	Joback Method
cpg	572.18	J/mol×K	752.02	Joback Method
cpg	587.02	J/mol×K	786.58	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=R344059&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

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