

(2R,5S)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca

Inchi:	InChI=1S/C13H22O2/c1-9-5-8-13(15-9)10(2)11(14)6-7-12(13,3)4/h9-10H,5-8H2,1-4H3
InchiKey:	UGLUSFJDQNOYMH-UHFFFAOYSA-N
Formula:	C13H22O2
SMILES:	CC1CCC2(O1)C(C)C(=O)CCC2(C)C
Mol. weight [g/mol]:	210.31
CAS:	66514-42-9

Physical Properties

Property code	Value	Unit	Source
gf	-103.43	kJ/mol	Joback Method
hf	-470.59	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	50.88	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.949		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1553.80		NIST Webbook
rinpol	1553.80		NIST Webbook
tb	613.31	K	Joback Method
tc	854.77	K	Joback Method
tf	392.18	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.45	J/molxK	613.31	Joback Method
cpg	533.06	J/molxK	653.55	Joback Method
cpg	554.45	J/molxK	693.80	Joback Method
cpg	574.86	J/molxK	734.04	Joback Method
cpg	594.54	J/molxK	774.28	Joback Method
cpg	613.74	J/molxK	814.52	Joback Method
cpg	632.72	J/molxK	854.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66514429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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