Dihydro-nor-dicyclopentadienyl propionate

Inchi: InChI=1S/C13H18O2/c1-2-13(14)15-12-7-8-6-11(12)10-5-3-4-9(8)10/h3-4,8-12H,2,5-7H2
InchiKey: BLBJUGKATXCWET-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCC(=O)OC1CC2CC1C1CC=CC21
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	9.35	kJ/mol	Joback Method
hf	-327.11	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	53.27	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.540		Crippen Method
mcvol	164.590	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1499.00		NIST Webbook
rinpol	1498.60		NIST Webbook
rinpol	1499.00		NIST Webbook
tb	587.44	K	Joback Method
tc	800.04	K	Joback Method
tf	351.01	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.66	J/mol×K	587.44	Joback Method
cpg	476.88	J/mol×K	622.87	Joback Method
cpg	494.86	J/mol×K	658.31	Joback Method
cpg	511.68	J/mol×K	693.74	Joback Method
cpg	527.43	J/mol×K	729.17	Joback Method
cpg	542.18	J/mol×K	764.61	Joback Method
cpg	556.00	J/mol×K	800.04	Joback Method

dvisc	0.0021683	Pa×s	351.01	Joback Method
dvisc	0.0021824	Pa×s	390.42	Joback Method
dvisc	0.0021939	Pa×s	429.82	Joback Method
dvisc	0.0022036	Pa×s	469.23	Joback Method
dvisc	0.0022118	Pa×s	508.63	Joback Method
dvisc	0.0022188	Pa×s	548.04	Joback Method
dvisc	0.0022249	Pa×s	587.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R129494&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
dvisc:	Dynamic viscosity
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