cis-5-Isopropenyl-2,2-dimethyltetrahydro-furan-3-acetate

Inchi: InChI=1S/C12H20O3/c1-8(2)11-6-10(7-14-9(3)13)12(4,5)15-11/h10-11H,1,6-7H2,2-5H3/t

InchiKey: ZIYIQFWIKYQOLB-MNOVXSKESA-N

Formula: C12H20O3

SMILES: C=C(C)C1CC(COC(C)=O)C(C)(C)O1

Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-174.95	kJ/mol	Joback Method
hf	-517.13	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.309		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1346.00		NIST Webbook
ripol	1831.00		NIST Webbook
tb	579.94	K	Joback Method
tc	785.99	K	Joback Method
tf	334.33	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.55	J/mol×K	579.94	Joback Method
cpg	484.38	J/mol×K	614.28	Joback Method
cpg	501.26	J/mol×K	648.62	Joback Method
cpg	517.30	J/mol×K	682.97	Joback Method
cpg	532.57	J/mol×K	717.31	Joback Method
cpg	547.17	J/mol×K	751.65	Joback Method
cpg	561.18	J/mol×K	785.99	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=R232590&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume