3-isopropenyl-2,2-dimethylcyclobutanemethyl acetate

Inchi: InChI=1S/C12H20O2/c1-8(2)11-6-10(12(11,4)5)7-14-9(3)13/h10-11H,1,6-7H2,2-5H3
InchiKey: XUCVWTVHEYSKFF-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=C(C)C1CC(COC(C)=O)C1(C)C
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-76.73	kJ/mol	Joback Method
hf	-378.97	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.788		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1281.00		NIST Webbook
ripol	1702.00		NIST Webbook
tb	548.72	K	Joback Method
tc	749.37	K	Joback Method
tf	311.28	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.40	J/mol×K	548.72	Joback Method
cpg	450.05	J/mol×K	582.16	Joback Method
cpg	466.75	J/mol×K	615.60	Joback Method
cpg	482.59	J/mol×K	649.05	Joback Method
cpg	497.66	J/mol×K	682.49	Joback Method
cpg	512.05	J/mol×K	715.93	Joback Method
cpg	525.84	J/mol×K	749.37	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=R504439&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