Isoprenyl pentanoate

Inchi: InChI=1S/C8H14O2/c1-4-5-6-8(9)10-7(2)3/h2,4-6H2,1,3H3
InchiKey: UFLBUFFOFIVMQT-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: C=C(C)OC(=O)CCCC
Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
gf	-138.15	kJ/mol	Joback Method
hf	-337.61	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	41.97	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.253		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
rinpol	1153.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1113.00		NIST Webbook
ripol	1365.00		NIST Webbook
tb	455.29	K	Joback Method
tc	637.18	K	Joback Method
tf	236.36	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.99	J/mol×K	455.29	Joback Method
cpg	274.81	J/mol×K	485.61	Joback Method
cpg	286.17	J/mol×K	515.92	Joback Method
cpg	297.08	J/mol×K	546.24	Joback Method
cpg	307.54	J/mol×K	576.55	Joback Method
cpg	317.57	J/mol×K	606.87	Joback Method

cpg	327.16	J/mol×K	637.18	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=R238281&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