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
af	0.5331		Cheméo Relay (1.0)
gf	-138.15	kJ/mol	Joback Method
hf	-453.40	kJ/mol	Cheméo Relay (1.0)
hfus	16.67	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Cheméo Relay (1.0)
ie	8.98	eV	Cheméo Relay (1.0)
log10ws	-1.85		Cheméo Relay (1.0)
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	420.11	K	Cheméo Relay (1.0)
tc	606.61	K	Cheméo Relay (1.0)
tf	199.93	K	Cheméo Relay (1.0)
vc	0.476	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R238281&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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