Hexanoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C14H26O2/c1-4-6-8-10-11-13(3)16-14(15)12-9-7-5-2/h10-11,13H,4-9,12H2,1-3
InchiKey: FCIRXSXAXUSWOF-ZHACJKMWSA-N
Formula: C14H26O2
SMILES: CCCCC=CC(C)OC(=O)CCCCC
Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-89.14	kJ/mol	Joback Method
hf	-465.15	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	55.48	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.245		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
tb	599.73	K	Joback Method
tc	776.52	K	Joback Method
tf	299.62	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.81	J/mol×K	599.73	Joback Method
cpg	564.64	J/mol×K	629.20	Joback Method
cpg	580.71	J/mol×K	658.66	Joback Method
cpg	596.06	J/mol×K	688.13	Joback Method
cpg	610.70	J/mol×K	717.59	Joback Method
cpg	624.64	J/mol×K	747.06	Joback Method
cpg	637.92	J/mol×K	776.52	Joback Method
dvisc	0.0035141	Pa×s	299.62	Joback Method

dvisc	0.0013453	Pa×s	349.64	Joback Method
dvisc	0.0006549	Pa×s	399.66	Joback Method
dvisc	0.0003742	Pa×s	449.68	Joback Method
dvisc	0.0002392	Pa×s	499.69	Joback Method
dvisc	0.0001658	Pa×s	549.71	Joback Method
dvisc	0.0001222	Pa×s	599.73	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=U299355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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