5-hexenyl 7-octenoate

Inchi: InChI=1S/C14H24O2/c1-3-5-7-9-10-12-14(15)16-13-11-8-6-4-2/h3-4H,1-2,5-13H2
InchiKey: LOWZNJSXSHGAHG-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: C=CCCCCCC(=O)OCCCCC=C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	8.76	kJ/mol	Joback Method
hf	-326.23	kJ/mol	Joback Method
hfus	32.24	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.022		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
ripol	1887.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1895.00		NIST Webbook
tb	589.37	K	Joback Method
tc	762.40	K	Joback Method
tf	316.18	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.55	J/mol×K	589.37	Joback Method
cpg	540.44	J/mol×K	618.21	Joback Method
cpg	555.64	J/mol×K	647.05	Joback Method
cpg	570.16	J/mol×K	675.89	Joback Method
cpg	584.02	J/mol×K	704.73	Joback Method

cpg	597.23	J/mol×K	733.56	Joback Method
cpg	609.82	J/mol×K	762.40	Joback Method
dvisc	0.0025438	Pa×s	316.18	Joback Method
dvisc	0.0012099	Pa×s	361.71	Joback Method
dvisc	0.0006795	Pa×s	407.24	Joback Method
dvisc	0.0004285	Pa×s	452.77	Joback Method
dvisc	0.0002940	Pa×s	498.31	Joback Method
dvisc	0.0002149	Pa×s	543.84	Joback Method
dvisc	0.0001648	Pa×s	589.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R313614&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume