3-Octenoic acid, pentyl ester

Inchi: InChI=1S/C13H24O2/c1-3-5-7-8-9-11-13(14)15-12-10-6-4-2/h8-9H,3-7,10-12H2,1-2H3/b
InchiKey: WKJSTVIOKRSKFL-CMDGGOBGSA-N
Formula: C13H24O2
SMILES: CCCCC=CCC(=O)OCCCCC
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-95.12	kJ/mol	Joback Method
hf	-439.23	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	53.65	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.856		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	577.29	K	Joback Method
tc	752.37	K	Joback Method
tf	303.35	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.80	J/mol×K	577.29	Joback Method
cpg	511.75	J/mol×K	606.47	Joback Method
cpg	527.01	J/mol×K	635.65	Joback Method
cpg	541.59	J/mol×K	664.83	Joback Method
cpg	555.52	J/mol×K	694.01	Joback Method
cpg	568.82	J/mol×K	723.19	Joback Method
cpg	581.49	J/mol×K	752.37	Joback Method
dvisc	0.0027407	Pa×s	303.35	Joback Method

dvisc	0.0012188	Pa×s	349.01	Joback Method
dvisc	0.0006538	Pa×s	394.66	Joback Method
dvisc	0.0003991	Pa×s	440.32	Joback Method
dvisc	0.0002673	Pa×s	485.98	Joback Method
dvisc	0.0001917	Pa×s	531.63	Joback Method
dvisc	0.0001450	Pa×s	577.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406125&Units=SI

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