6-Methyl-4-heptenyl pentanoate

Inchi: InChI=1S/C13H24O2/c1-4-5-10-13(14)15-11-8-6-7-9-12(2)3/h7,9,12H,4-6,8,10-11H2,1-3
InchiKey: GSZZRNCIEMCQMD-VQHVLOKHSA-N
Formula: C13H24O2
SMILES: CCCCC(=O)OCCCC=CC(C)C
Mol. weight [g/mol]: 212.33
CAS: 1215128-07-6

Physical Properties

Property code	Value	Unit	Source
gf	-97.56	kJ/mol	Joback Method
hf	-444.51	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	53.26	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.712		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	576.85	K	Joback Method
tc	755.04	K	Joback Method
tf	288.35	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.13	J/mol×K	576.85	Joback Method
cpg	570.51	J/mol×K	725.34	Joback Method
cpg	557.00	J/mol×K	695.64	Joback Method
cpg	542.83	J/mol×K	665.95	Joback Method
cpg	527.97	J/mol×K	636.25	Joback Method
cpg	512.41	J/mol×K	606.55	Joback Method
cpg	583.37	J/mol×K	755.04	Joback Method

dvisc	0.0001357	Pa×s	576.85	Joback Method
dvisc	0.0001836	Pa×s	528.77	Joback Method
dvisc	0.0002639	Pa×s	480.68	Joback Method
dvisc	0.0004110	Pa×s	432.60	Joback Method
dvisc	0.0007154	Pa×s	384.52	Joback Method
dvisc	0.0014586	Pa×s	336.43	Joback Method
dvisc	0.0037720	Pa×s	288.35	Joback Method

Sources

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=C1215128076&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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