2-Heptenoic acid, heptyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-86.70	kJ/mol	Joback Method
hf	-459.87	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.246		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	600.17	K	Joback Method
tc	774.06	K	Joback Method
tf	314.62	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.45	J/mol×K	600.17	Joback Method
cpg	622.98	J/mol×K	745.08	Joback Method
cpg	609.24	J/mol×K	716.10	Joback Method
cpg	594.83	J/mol×K	687.12	Joback Method
cpg	579.75	J/mol×K	658.13	Joback Method
cpg	563.96	J/mol×K	629.15	Joback Method
cpg	636.08	J/mol×K	774.06	Joback Method
dvisc	0.0001309	Pa×s	600.17	Joback Method

dvisc	0.0001737	Pa×s	552.58	Joback Method
dvisc	0.0002432	Pa×s	504.99	Joback Method
dvisc	0.0003653	Pa×s	457.40	Joback Method
dvisc	0.0006028	Pa×s	409.80	Joback Method
dvisc	0.0011349	Pa×s	362.21	Joback Method
dvisc	0.0025872	Pa×s	314.62	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=U406093&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