Allyl 2-heptenoate

Inchi: InChI=1S/C10H16O2/c1-3-5-6-7-8-10(11)12-9-4-2/h4,7-8H,2-3,5-6,9H2,1H3/b8-7+
InchiKey: VHJIZSCKFCIYGY-BQYQJAHWSA-N
Formula: C10H16O2
SMILES: C=CCOC(=O)C=CCCCC
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-32.54	kJ/mol	Joback Method
hf	-251.88	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	46.30	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1454.00		NIST Webbook
tb	505.33	K	Joback Method
tc	688.59	K	Joback Method
tf	267.78	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.46	J/mol×K	505.33	Joback Method
cpg	345.70	J/mol×K	535.87	Joback Method
cpg	358.33	J/mol×K	566.42	Joback Method
cpg	370.39	J/mol×K	596.96	Joback Method
cpg	381.88	J/mol×K	627.50	Joback Method
cpg	392.82	J/mol×K	658.05	Joback Method

cpg	403.24	J/mol×K	688.59	Joback Method
dvisc	0.0028123	Pa×s	267.78	Joback Method
dvisc	0.0013463	Pa×s	307.37	Joback Method
dvisc	0.0007625	Pa×s	346.96	Joback Method
dvisc	0.0004852	Pa×s	386.55	Joback Method
dvisc	0.0003358	Pa×s	426.15	Joback Method
dvisc	0.0002474	Pa×s	465.74	Joback Method
dvisc	0.0001912	Pa×s	505.33	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=R409384&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume