n-Heptyl acrylate

Other names:	2-Propenoic acid, heptyl ester
	Acrylic acid, heptyl ester
	ENT 15748
	Heptyl acrylate
Inchi:	InChI=1S/C10H18O2/c1-3-5-6-7-8-9-12-10(11)4-2/h4H,2-3,5-9H2,1H3
InchiKey:	SCFQUKBBGYTJNC-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CC(=O)OCCCCCCC
Mol. weight [g/mol]:	170.25
CAS:	2499-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-112.76	kJ/mol	Joback Method
hf	-369.10	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	46.34	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1173.00		NIST Webbook
ripol	1489.00		NIST Webbook
tb	501.17	K	Joback Method
tc	676.68	K	Joback Method
tf	272.86	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.85	J/mol×K	501.17	Joback Method
cpg	363.46	J/mol×K	530.42	Joback Method
cpg	376.52	J/mol×K	559.67	Joback Method

cpg	389.06	J/mol×K	588.93	Joback Method
cpg	401.07	J/mol×K	618.18	Joback Method
cpg	412.57	J/mol×K	647.43	Joback Method
cpg	423.57	J/mol×K	676.68	Joback Method
dvisc	0.0030420	Pa×s	272.86	Joback Method
dvisc	0.0015143	Pa×s	310.91	Joback Method
dvisc	0.0008777	Pa×s	348.96	Joback Method
dvisc	0.0005663	Pa×s	387.01	Joback Method
dvisc	0.0003952	Pa×s	425.07	Joback Method
dvisc	0.0002926	Pa×s	463.12	Joback Method
dvisc	0.0002268	Pa×s	501.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57305e+01
Coeff. B	-4.51965e+03
Coeff. C	-7.63250e+01
Temperature range (K), min.	368.99
Temperature range (K), max.	510.11

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2499583&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor 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