n-Propyl acrylate

Other names:	1-Propyl acrylate
	2-Propenoic acid, propyl ester
	Acrylic acid, propyl ester
	Propyl 2-propenoate
	Propylacrylate
Inchi:	InChI=1S/C6H10O2/c1-3-5-8-6(7)4-2/h4H,2-3,5H2,1H3
InchiKey:	PNXMTCDJUBJHQJ-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	C=CC(=O)OCCC
Mol. weight [g/mol]:	114.14
CAS:	925-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-146.44	kJ/mol	Joback Method
hf	-286.54	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	37.44	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	748.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	779.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1080.00		NIST Webbook
ripol	1074.00		NIST Webbook
ripol	1078.00		NIST Webbook
tb	409.65	K	Joback Method
tc	590.97	K	Joback Method
tf	227.78	K	Joback Method

vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.15	J/mol×K	590.97	Joback Method
cpg	184.90	J/mol×K	409.65	Joback Method
cpg	194.08	J/mol×K	439.87	Joback Method
cpg	202.94	J/mol×K	470.09	Joback Method
cpg	211.47	J/mol×K	500.31	Joback Method
cpg	219.68	J/mol×K	530.53	Joback Method
cpg	227.57	J/mol×K	560.75	Joback Method
dvisc	0.0002688	Pa×s	409.65	Joback Method
dvisc	0.0026729	Pa×s	227.78	Joback Method
dvisc	0.0014557	Pa×s	258.09	Joback Method
dvisc	0.0009008	Pa×s	288.40	Joback Method
dvisc	0.0006108	Pa×s	318.72	Joback Method
dvisc	0.0004430	Pa×s	349.03	Joback Method
dvisc	0.0003382	Pa×s	379.34	Joback Method
hvapt	37.90	kJ/mol	341.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.50295e+01
Coeff. B	-7.91265e+03
Coeff. C	-1.02435e+01
Coeff. D	5.98168e-06
Temperature range (K), min.	273.15
Temperature range (K), max.	569.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1177.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C925600&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1177
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
hvapt:	Enthalpy of vaporization at a given temperature
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