2-Propenoic acid, octyl ester

Other names:	Acrylic acid, octyl ester
	ENT 3827
	Octyl Acrylate
	n-Octyl acrylate
Inchi:	InChI=1S/C11H20O2/c1-3-5-6-7-8-9-10-13-11(12)4-2/h4H,2-3,5-10H2,1H3
InchiKey:	ANISOHQJBAQUQP-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	C=CC(=O)OCCCCCCCC
Mol. weight [g/mol]:	184.28
CAS:	2499-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-104.34	kJ/mol	Joback Method
hf	-389.74	kJ/mol	Joback Method
hfus	25.75	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1295.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1590.00		NIST Webbook
tb	524.05	K	Joback Method
tc	698.08	K	Joback Method
tf	284.13	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.25	J/mol×K	698.08	Joback Method
cpg	396.19	J/mol×K	524.05	Joback Method
cpg	410.62	J/mol×K	553.05	Joback Method
cpg	424.47	J/mol×K	582.06	Joback Method
cpg	437.74	J/mol×K	611.06	Joback Method
cpg	450.46	J/mol×K	640.07	Joback Method
cpg	462.62	J/mol×K	669.07	Joback Method
dvisc	0.0002102	Pa×s	524.05	Joback Method
dvisc	0.0029982	Pa×s	284.13	Joback Method
dvisc	0.0014650	Pa×s	324.12	Joback Method
dvisc	0.0008378	Pa×s	364.10	Joback Method
dvisc	0.0005351	Pa×s	404.09	Joback Method
dvisc	0.0003706	Pa×s	444.08	Joback Method
dvisc	0.0002727	Pa×s	484.06	Joback Method
hvapt	56.20	kJ/mol	415.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65377e+01
Coeff. B	-4.97929e+03
Coeff. C	-8.36470e+01
Temperature range (K), min.	390.06
Temperature range (K), max.	527.19

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2499594&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
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