2-Propenoic acid, 2-methyl-, octyl ester

Other names:	Octyl methacrylate
	n-Octyl methacrylate
	Methacrylic acid, octyl ester
Inchi:	InChI=1S/C12H22O2/c1-4-5-6-7-8-9-10-14-12(13)11(2)3/h2,4-10H2,1,3H3
InchiKey:	NZIDBRBFGPQCRY-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	C=C(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]:	198.30
CAS:	2157-01-9

Physical Properties

Property code	Value	Unit	Source
gf	-104.47	kJ/mol	Joback Method
hf	-420.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	1356.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1639.00		NIST Webbook
tb	546.81	K	Joback Method
tc	722.17	K	Joback Method
tf	230.30 ± 0.20	K	NIST Webbook
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.15	J/mol×K	546.81	Joback Method
cpg	459.52	J/mol×K	576.04	Joback Method

cpg	474.25	J/mol×K	605.26	Joback Method
cpg	488.35	J/mol×K	634.49	Joback Method
cpg	501.84	J/mol×K	663.72	Joback Method
cpg	514.73	J/mol×K	692.95	Joback Method
cpg	527.04	J/mol×K	722.17	Joback Method
hfust	24.09	kJ/mol	230.30	NIST Webbook
hvapt	55.60	kJ/mol	448.50	NIST Webbook

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=C2157019&Units=SI

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
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