2-Propenoic acid, 2-methyl-, hexyl ester

Other names:	Methacrylic acid, hexyl ester
	ENT 25419
	Hexyl Methacrylate
	Hexyl 2-methyl-2-propenoate
	n-Hexyl methacrylate
	Methacrylic acid n-hexyl ester
Inchi:	InChI=1S/C10H18O2/c1-4-5-6-7-8-12-10(11)9(2)3/h2,4-8H2,1,3H3
InchiKey:	LNCPIMCVTKXXOY-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=C(C)C(=O)OCCCCCC
Mol. weight [g/mol]:	170.25
CAS:	142-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-121.31	kJ/mol	Joback Method
hf	-378.89	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1164.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1439.00		NIST Webbook
tb	501.05	K	Joback Method
tc	679.59	K	Joback Method

tf	258.90	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.27	J/mol×K	649.83	Joback Method
cpg	349.71	J/mol×K	501.05	Joback Method
cpg	363.52	J/mol×K	530.81	Joback Method
cpg	376.77	J/mol×K	560.56	Joback Method
cpg	389.47	J/mol×K	590.32	Joback Method
cpg	401.64	J/mol×K	620.08	Joback Method
cpg	424.39	J/mol×K	679.59	Joback Method
hvapt	50.50	kJ/mol	414.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C142096&Units=SI
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
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

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