2-Propenoic acid, 2-methyl-, heptyl ester

Other names: Heptyl methacrylate
Inchi: InChI=1S/C11H20O2/c1-4-5-6-7-8-9-13-11(12)10(2)3/h2,4-9H2,1,3H3
InchiKey: MDNFYIAABKQDML-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: C=C(C)C(=O)OCCCCCCC
Mol. weight [g/mol]: 184.28
CAS: 5459-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-112.89	kJ/mol	Joback Method
hf	-399.53	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	48.65	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1215.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1257.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1538.00		NIST Webbook
tb	523.93	K	Joback Method
tc	700.83	K	Joback Method
tf	270.17	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.02	J/mol×K	523.93	Joback Method

cpg	410.66	J/mol×K	553.41	Joback Method
cpg	424.70	J/mol×K	582.90	Joback Method
cpg	438.14	J/mol×K	612.38	Joback Method
cpg	451.01	J/mol×K	641.86	Joback Method
cpg	463.32	J/mol×K	671.35	Joback Method
cpg	475.06	J/mol×K	700.83	Joback Method

Sources

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=C5459370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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