2-Propenoic acid, 6-methylheptyl ester

Other names: 6-Methylheptyl 2-propenoate
6-Methylheptyl prop-2-enoate
6-methylheptyl acrylate
Inchi: InChI=1S/C11H20O2/c1-4-11(12)13-9-7-5-6-8-10(2)3/h4,10H,1,5-9H2,2-3H3
InchiKey: DXPPIEDUBFUSEZ-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: C=CC(=O)OCCCCCC(C)C
Mol. weight [g/mol]: 184.28
CAS: 54774-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-106.78	kJ/mol	Joback Method
hf	-395.02	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	48.18	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.932		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1232.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1232.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1480.00		NIST Webbook
tb	523.61	K	Joback Method
tc	701.05	K	Joback Method
tf	269.13	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	396.43	J/mol×K	523.61	Joback Method
cpg	464.30	J/mol×K	671.47	Joback Method
cpg	451.91	J/mol×K	641.90	Joback Method
cpg	438.94	J/mol×K	612.33	Joback Method
cpg	425.37	J/mol×K	582.76	Joback Method
cpg	411.21	J/mol×K	553.18	Joback Method
cpg	476.13	J/mol×K	701.05	Joback Method
dvisc	0.0001982	Pa×s	523.61	Joback Method
dvisc	0.0002632	Pa×s	481.20	Joback Method
dvisc	0.0003694	Pa×s	438.78	Joback Method
dvisc	0.0005575	Pa×s	396.37	Joback Method
dvisc	0.0009284	Pa×s	353.96	Joback Method
dvisc	0.0017765	Pa×s	311.54	Joback Method
dvisc	0.0041707	Pa×s	269.13	Joback Method

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=C54774913&Units=SI

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
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