2-Propenoic acid, 2-methyl-, 4-methylpentyl ester

Other names: Isohexyl methacrylate
4-methylpentyl methacrylate
Inchi: InChI=1S/C10H18O2/c1-8(2)6-5-7-12-10(11)9(3)4/h8H,3,5-7H2,1-2,4H3
InchiKey: TZCGFWIYMJNJIO-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: C=C(C)C(=O)OCCCC(C)C
Mol. weight [g/mol]: 170.25
CAS: 7766-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-123.75	kJ/mol	Joback Method
hf	-384.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
ripol	1370.00		NIST Webbook
tb	500.61	K	Joback Method
tc	682.86	K	Joback Method
tf	243.90	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.92	J/mol×K	500.61	Joback Method
cpg	364.09	J/mol×K	530.98	Joback Method
cpg	377.66	J/mol×K	561.36	Joback Method
cpg	390.66	J/mol×K	591.73	Joback Method
cpg	403.09	J/mol×K	622.11	Joback Method
cpg	414.96	J/mol×K	652.48	Joback Method

cpg	426.29	J/mol×K	682.86	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=C7766612&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume