2-Propenoic acid, 2-methyl-, 3-methylbutyl ester

Other names: 3-Methylbutyl methacrylate
Isopentyl methacrylate
3-Methylbutyl trichloroacetate

Inchi: InChI=1S/C9H16O2/c1-7(2)5-6-11-9(10)8(3)4/h7H,3,5-6H2,1-2,4H3

InchiKey: ULYIFEQRRINMJQ-UHFFFAOYSA-N

Formula: C9H16O2

SMILES: C=C(C)C(=O)OCCC(C)C

Mol. weight [g/mol]: 156.22

CAS: 7336-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-132.17	kJ/mol	Joback Method
hf	-363.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	43.81	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1027.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1043.50		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1043.50		NIST Webbook
rinpol	1019.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1281.00		NIST Webbook
tb	477.73	K	Joback Method
tc	661.84	K	Joback Method
tf	232.63	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.50	J/mol×K	477.73	Joback Method
cpg	318.73	J/mol×K	508.42	Joback Method
cpg	331.41	J/mol×K	539.10	Joback Method
cpg	343.57	J/mol×K	569.79	Joback Method
cpg	355.20	J/mol×K	600.47	Joback Method
cpg	366.31	J/mol×K	631.16	Joback Method
cpg	376.93	J/mol×K	661.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7336278&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
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