3-METHYL,2-BUTENOIC ACID,ISOPROPYL ESTER

Other names: 2-Butenoic acid, 3-methyl, 1-methylethyl ester
Crotonic acid, 3-methyl-, isopropyl ester
Isopropyl 3-methyl-2-butenoate
Isopropyl 3-methylbut-2-enoate

Inchi: InChI=1S/C8H14O2/c1-6(2)5-8(9)10-7(3)4/h5,7H,1-4H3

InchiKey: QQVQBUXUAZCLLZ-UHFFFAOYSA-N

Formula: C8H14O2

SMILES: CC(C)=CC(=O)OC(C)C

Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
hf	-451.06	kJ/mol	Cheméo Relay (1.0)
hfus	14.63	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Cheméo Relay (1.0)
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-2.28		Cheméo Relay (1.0)
logp	1.904		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	409.82	K	Cheméo Relay (1.0)
tc	603.18	K	Cheméo Relay (1.0)
tf	241.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.35	J/mol×K	462.33	Joback Method
cpg	275.79	J/mol×K	494.15	Joback Method
cpg	287.69	J/mol×K	525.98	Joback Method
cpg	299.05	J/mol×K	557.80	Joback Method
cpg	309.90	J/mol×K	589.63	Joback Method
cpg	320.24	J/mol×K	621.45	Joback Method
cpg	330.09	J/mol×K	653.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25859512&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point