

3-Methyl,2-butenic acid, isopropyl ester

Other names:	Isopropyl 3-methyl-2-butenate 2-Butenoic acid, 3-methyl, 1-methylethyl ester Crotonic acid, 3-methyl-, isopropyl ester 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
CAS:	25859-51-2

Physical Properties

Property code	Value	Unit	Source
gf	-148.21	kJ/mol	Joback Method
hf	-351.10	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	50.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.00		Crippen Method
logp	1.904		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	940.00		NIST Webbook
tb	462.33	K	Joback Method
tc	653.28	K	Joback Method
tf	218.04	K	Joback Method
vc	0.482	m3/kmol	Joback Method

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

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=C25859512&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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