

3-Methyl-2-butenic acid, 3-methylbut-2-enyl ester

Other names:	3-methylbut-2-en-1-yl 3-methylbut-2-enoate 3-methyl-2-butenyl 3-methyl-2-butenolate
Inchi:	InChI=1S/C10H16O2/c1-8(2)5-6-12-10(11)7-9(3)4/h5,7H,6H2,1-4H3
InchiKey:	CBERZXRMIOEKPW-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)=CCOC(=O)C=C(C)C
Mol. weight [g/mol]:	168.23
CAS:	72779-06-7

Physical Properties

Property code	Value	Unit	Source
gf	-57.26	kJ/mol	Joback Method
hf	-279.67	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	47.09	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1234.70		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1234.70		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1245.00		NIST Webbook
tb	512.57	K	Joback Method
tc	707.11	K	Joback Method
tf	236.54	K	Joback Method
vc	0.582	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.83	J/molxK	512.57	Joback Method

cpg	346.67	J/mol×K	544.99	Joback Method
cpg	359.82	J/mol×K	577.42	Joback Method
cpg	372.30	J/mol×K	609.84	Joback Method
cpg	384.14	J/mol×K	642.27	Joback Method
cpg	395.38	J/mol×K	674.69	Joback Method
cpg	406.04	J/mol×K	707.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C72779067&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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