

3-methyl-3-butenyl 2-methylcrotonate

Other names:	(E)-3-Methylbut-3-en-1-yl 2-methylbut-2-enoate
Inchi:	InChI=1S/C10H16O2/c1-5-9(4)10(11)12-7-6-8(2)3/h5H,2,6-7H2,1,3-4H3/b9-5+
InchiKey:	LMPCYQLIAVCCCL-WEVVVXLNSA-N
Formula:	C10H16O2
SMILES:	<chem>C=C(C)CCOC(=O)C(C)=CC</chem>
Mol. weight [g/mol]:	168.23
CAS:	83783-87-3

Physical Properties

Property code	Value	Unit	Source
gf	-49.64	kJ/mol	Joback Method
hf	-271.46	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	46.46	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1204.80		NIST Webbook
rinpol	1204.80		NIST Webbook
tb	505.09	K	Joback Method
tc	694.94	K	Joback Method
tf	239.86	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.18	J/molxK	505.09	Joback Method
cpg	345.83	J/molxK	536.73	Joback Method
cpg	358.83	J/molxK	568.37	Joback Method
cpg	371.21	J/molxK	600.02	Joback Method
cpg	382.99	J/molxK	631.66	Joback Method
cpg	394.19	J/molxK	663.30	Joback Method

Sources

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=C83783873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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