2-methylallyl 2-methylcrotonate

Other names: (E)-2-Methylallyl 2-methylbut-2-enoate
Inchi: InChI=1S/C9H14O2/c1-5-8(4)9(10)11-6-7(2)3/h5H,2,6H2,1,3-4H3/b8-5+
InchiKey: PNRCWIZNCBKLMH-VMPITWQZSA-N
Formula: C9H14O2
SMILES: C=C(C)COC(=O)C(C)=CC
Mol. weight [g/mol]: 154.21
CAS: 61692-82-8

Physical Properties

Property code	Value	Unit	Source
gf	-58.06	kJ/mol	Joback Method
hf	-250.82	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	44.23	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.072		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
tb	482.21	K	Joback Method
tc	674.32	K	Joback Method
tf	228.59	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.32	J/mol×K	482.21	Joback Method
cpg	301.01	J/mol×K	514.23	Joback Method
cpg	313.11	J/mol×K	546.25	Joback Method
cpg	324.62	J/mol×K	578.26	Joback Method
cpg	335.58	J/mol×K	610.28	Joback Method
cpg	346.00	J/mol×K	642.30	Joback Method

cpg	355.89	J/mol×K	674.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61692828&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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