3,3-Dimethylbutan-2-yl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C11H20O2/c1-7-8(2)10(12)13-9(3)11(4,5)6/h7,9H,1-6H3/b8-7+

InchiKey: VCVVPZCHFOZXNS-BQYQJAHWSA-N

Formula: C11H20O2

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

Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-120.11	kJ/mol	Joback Method
hf	-421.77	kJ/mol	Joback Method
hfus	14.99	kJ/mol	Joback Method
hvap	47.59	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.930		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1184.00		NIST Webbook
rinpol	1184.00		NIST Webbook
tb	527.74	K	Joback Method
tc	723.38	K	Joback Method
tf	254.27	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.46	J/mol×K	527.74	Joback Method
cpg	416.69	J/mol×K	560.35	Joback Method
cpg	432.06	J/mol×K	592.95	Joback Method
cpg	446.59	J/mol×K	625.56	Joback Method
cpg	460.32	J/mol×K	658.17	Joback Method
cpg	473.29	J/mol×K	690.78	Joback Method
cpg	485.54	J/mol×K	723.38	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=U373759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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