3-Oxobutan-2-yl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C9H14O3/c1-5-6(2)9(11)12-8(4)7(3)10/h5,8H,1-4H3/b6-5+
InchiKey: PNUCZORMJRDQRQ-AATRIKPKSA-N
Formula: C9H14O3
SMILES: CC=C(C)C(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 170.21

Physical Properties

Property code	Value	Unit	Source
gf	-268.71	kJ/mol	Joback Method
hf	-484.32	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	51.18	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.473		Crippen Method
mcvol	142.380	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1198.00		NIST Webbook
tb	539.08	K	Joback Method
tc	737.09	K	Joback Method
tf	279.24	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.07	J/mol×K	539.08	Joback Method
cpg	337.61	J/mol×K	572.08	Joback Method
cpg	349.53	J/mol×K	605.08	Joback Method
cpg	360.85	J/mol×K	638.08	Joback Method
cpg	371.59	J/mol×K	671.08	Joback Method
cpg	381.75	J/mol×K	704.08	Joback Method
cpg	391.36	J/mol×K	737.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373719&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

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