3-Methylbut-2-enoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C10H18O2/c1-7(2)6-10(11)12-9(5)8(3)4/h6,8-9H,1-5H3
InchiKey: KJAJVDYSLRBEOK-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(C)=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-133.81	kJ/mol	Joback Method
hf	-397.66	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.540		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1148.00		NIST Webbook
tb	507.65	K	Joback Method
tc	698.35	K	Joback Method
tf	225.58	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.05	J/mol×K	507.65	Joback Method
cpg	365.81	J/mol×K	539.43	Joback Method
cpg	379.90	J/mol×K	571.22	Joback Method
cpg	393.33	J/mol×K	603.00	Joback Method
cpg	406.12	J/mol×K	634.78	Joback Method
cpg	418.29	J/mol×K	666.57	Joback Method
cpg	429.86	J/mol×K	698.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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