2-methylallyl 2-methylbutyrate

Other names: 2-Methylallyl 2-methylbutanoate
Inchi: InChI=1S/C9H16O2/c1-5-8(4)9(10)11-6-7(2)3/h8H,2,5-6H2,1,3-4H3
InchiKey: FSSVRXASHHVANB-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: C=C(C)COC(=O)C(C)CC
Mol. weight [g/mol]: 156.22
CAS: 83783-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-132.17	kJ/mol	Joback Method
hf	-363.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	43.81	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1018.10		NIST Webbook
rinpol	1018.10		NIST Webbook
tb	477.73	K	Joback Method
tc	661.84	K	Joback Method
tf	232.63	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.50	J/mol×K	477.73	Joback Method
cpg	318.73	J/mol×K	508.42	Joback Method
cpg	331.41	J/mol×K	539.10	Joback Method
cpg	343.57	J/mol×K	569.79	Joback Method
cpg	355.20	J/mol×K	600.47	Joback Method
cpg	366.31	J/mol×K	631.16	Joback Method

cpg	376.93	J/mol×K	661.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83783908&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