3-methyl-but-3-en-1-yl 3-methyl-but-2-enoate

Inchi: InChI=1S/C10H16O2/c1-8(2)5-6-12-10(11)7-9(3)4/h7H,1,5-6H2,2-4H3
InchiKey: GRTNNHGFEQUXEO-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: C=C(C)CCOC(=O)C=C(C)C
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-49.64	kJ/mol	Joback Method
hf	-271.46	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	46.46	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1195.00		NIST Webbook
tb	505.09	K	Joback Method
tc	694.94	K	Joback Method
tf	239.86	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.18	J/mol×K	505.09	Joback Method
cpg	345.83	J/mol×K	536.73	Joback Method
cpg	358.83	J/mol×K	568.37	Joback Method
cpg	371.21	J/mol×K	600.02	Joback Method
cpg	382.99	J/mol×K	631.66	Joback Method
cpg	394.19	J/mol×K	663.30	Joback Method
cpg	404.83	J/mol×K	694.94	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=R279455&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