3-Methyl-2-buten-1-yl 2-methylbutanoate

Inchi: InChI=1S/C10H18O2/c1-5-9(4)10(11)12-7-6-8(2)3/h6,9H,5,7H2,1-4H3
InchiKey: SPZJCVIOUQJWGX-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCC(C)C(=O)OCC=C(C)C
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
hf	-488.41	kJ/mol	Cheméo Relay (1.0)
hfus	19.81	kJ/mol	Joback Method
hvap	55.12	kJ/mol	Cheméo Relay (1.0)
ie	8.75	eV	Cheméo Relay (1.0)
log10ws	-2.77		Cheméo Relay (1.0)
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
rinpol	1146.00		NIST Webbook
rinpol	1138.00		NIST Webbook
tb	449.05	K	Cheméo Relay (1.0)
tc	641.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.82	J/mol×K	508.09	Joback Method
cpg	365.21	J/mol×K	539.21	Joback Method
cpg	378.95	J/mol×K	570.33	Joback Method
cpg	392.08	J/mol×K	601.46	Joback Method
cpg	404.60	J/mol×K	632.58	Joback Method
cpg	416.53	J/mol×K	663.70	Joback Method
cpg	427.88	J/mol×K	694.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R342013&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature