

3-Methylbut-2-en-1-yl 3-methylbut-2-enoate

Other names:	3-methylbut-2-en-1-yl 3-methylbut-2-enoate 3-methyl-2-butenyl 3-methyl-2-butenolate
Inchi:	InChI=1S/C10H16O2/c1-8(2)5-6-12-10(11)7-9(3)4/h5,7H,6H2,1-4H3
InchiKey:	CBERZXRMIOEKPW-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)=CCOC(=O)C=C(C)C
Mol. weight [g/mol]:	168.24

Physical Properties

Property code	Value	Unit	Source
hfus	22.23	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Cheméo Relay (1.0)
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1234.70		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1234.70		NIST Webbook
tb	475.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.83	J/mol×K	512.57	Joback Method
cpg	346.67	J/mol×K	544.99	Joback Method
cpg	359.82	J/mol×K	577.42	Joback Method
cpg	372.30	J/mol×K	609.84	Joback Method
cpg	384.14	J/mol×K	642.27	Joback Method
cpg	395.38	J/mol×K	674.69	Joback Method
cpg	406.04	J/mol×K	707.11	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72779067&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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