

3-Methyl-2-butenolic acid, 2-pentyl ester

Other names:	2-Pentanol, (E)-3-methyl-2-butenolate
Inchi:	InChI=1S/C10H18O2/c1-5-6-9(4)12-10(11)7-8(2)3/h7,9H,5-6H2,1-4H3
InchiKey:	XVLXJODMJPDWEI-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCCC(C)OC(=O)C=C(C)C
Mol. weight [g/mol]:	170.25
CAS:	150462-84-3

Physical Properties

Property code	Value	Unit	Source
gf	-131.37	kJ/mol	Joback Method
hf	-392.38	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.684		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1049.00		NIST Webbook
rinpol	1049.00		NIST Webbook
tb	508.09	K	Joback Method
tc	694.82	K	Joback Method
tf	240.58	K	Joback Method
vc	0.595	m3/kmol	Joback Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C150462843&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

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