

2-Hydroxy-2-methyl-but-3-enyl 2-methyl-2(Z)-butenoate

Other names:	(Z)-2-Hydroxy-2-methylbut-3-en-1-yl 2-methylbut-2-enoate
Inchi:	InChI=1S/C10H16O3/c1-5-8(3)9(11)13-7-10(4,12)6-2/h5-6,12H,2,7H2,1,3-4H3/b8-5+
InchiKey:	QQSQGJPTALGCLH-VMPITWQZSA-N
Formula:	C10H16O3
SMILES:	C=CC(C)(O)COC(=O)C(C)=CC
Mol. weight [g/mol]:	184.23
CAS:	80758-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-175.07	kJ/mol	Joback Method
hf	-422.65	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	61.76	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.433		Crippen Method
mcvol	156.470	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1250.40		NIST Webbook
tb	594.16	K	Joback Method
tc	781.09	K	Joback Method
tf	317.06	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.67	J/molxK	594.16	Joback Method
cpg	402.54	J/molxK	625.31	Joback Method
cpg	413.75	J/molxK	656.47	Joback Method
cpg	424.34	J/molxK	687.62	Joback Method
cpg	434.33	J/molxK	718.78	Joback Method
cpg	443.76	J/molxK	749.93	Joback Method
cpg	452.68	J/molxK	781.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80758674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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