

3-Methylbut-2-en-1-yl pivalate

Inchi:	InChI=1S/C10H18O2/c1-8(2)6-7-12-9(11)10(3,4)5/h6H,7H2,1-5H3
InchiKey:	AXJGWZOWJMGIEF-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC(C)=CCOC(=O)C(C)(C)C
Mol. weight [g/mol]:	170.25
CAS:	211429-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-126.09	kJ/mol	Joback Method
hf	-395.85	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	45.75	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1140.90		NIST Webbook
tb	505.30	K	Joback Method
tc	699.32	K	Joback Method
tf	258.00	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.60	J/mol×K	505.30	Joback Method
cpg	368.69	J/mol×K	537.64	Joback Method
cpg	382.99	J/mol×K	569.97	Joback Method
cpg	396.52	J/mol×K	602.31	Joback Method
cpg	409.32	J/mol×K	634.65	Joback Method
cpg	421.42	J/mol×K	666.98	Joback Method
cpg	432.86	J/mol×K	699.32	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=C211429719&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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