

4-Pentenoic acid, 2-methyl-, isobutyl ester

Inchi:	InChI=1S/C10H18O2/c1-5-6-9(4)10(11)12-7-8(2)3/h5,8-9H,1,6-7H2,2-4H3
InchiKey:	WBOXHCVWWIJOLN-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CCC(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-117.64	kJ/mol	Joback Method
hf	-379.66	kJ/mol	Joback Method
hfus	16.12	kJ/mol	Joback Method
hvap	45.56	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.398		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinsol	1080.00		NIST Webbook
tb	500.29	K	Joback Method
tc	683.12	K	Joback Method
tf	242.86	K	Joback Method
vc	0.589	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.27	J/molxK	500.29	Joback Method
cpg	364.58	J/molxK	530.76	Joback Method
cpg	378.29	J/molxK	561.23	Joback Method
cpg	391.42	J/molxK	591.71	Joback Method
cpg	403.96	J/molxK	622.18	Joback Method
cpg	415.93	J/molxK	652.65	Joback Method
cpg	427.34	J/molxK	683.12	Joback Method
dvisc	0.0064238	Paxs	242.86	Joback Method
dvisc	0.0023439	Paxs	285.76	Joback Method

dvisc	0.0011128	Paxs	328.67	Joback Method
dvisc	0.0006275	Paxs	371.57	Joback Method
dvisc	0.0003984	Paxs	414.48	Joback Method
dvisc	0.0002754	Paxs	457.38	Joback Method
dvisc	0.0002029	Paxs	500.29	Joback Method

Sources

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=U406105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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