

Isovaleric acid, 3-methylbutyl-2 ester

Inchi:	InChI=1S/C10H20O2/c1-7(2)6-10(11)12-9(5)8(3)4/h7-9H,6H2,1-5H3
InchiKey:	QHNMTYMWSUDOHU-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CC(C)CC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	172.26

Physical Properties

Property code	Value	Unit	Source
gf	-207.92	kJ/mol	Joback Method
hf	-510.37	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	45.85	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.620		Crippen Method
mvol	159.200	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
tb	503.17	K	Joback Method
tc	686.24	K	Joback Method
tf	229.62	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.71	J/molxK	503.17	Joback Method
cpg	383.96	J/molxK	533.68	Joback Method
cpg	398.59	J/molxK	564.19	Joback Method
cpg	412.61	J/molxK	594.71	Joback Method
cpg	426.03	J/molxK	625.22	Joback Method
cpg	438.85	J/molxK	655.73	Joback Method
cpg	451.08	J/molxK	686.24	Joback Method
dvisc	0.0114324	Paxs	229.62	Joback Method

dvisc	0.0032727	Paxs	275.21	Joback Method
dvisc	0.0013368	Paxs	320.80	Joback Method
dvisc	0.0006824	Paxs	366.39	Joback Method
dvisc	0.0004042	Paxs	411.99	Joback Method
dvisc	0.0002658	Paxs	457.58	Joback Method
dvisc	0.0001885	Paxs	503.17	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=U360649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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