

3,4-Dimethylpentanoic acid

Inchi:	InChI=1S/C7H14O2/c1-5(2)6(3)4-7(8)9/h5-6H,4H2,1-3H3,(H,8,9)
InchiKey:	GETAKGOKCSRVLZ-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CC(C)C(C)CC(=O)O
Mol. weight [g/mol]:	130.18

Physical Properties

Property code	Value	Unit	Source
gf	-262.56	kJ/mol	Joback Method
hf	-463.18	kJ/mol	Joback Method
hfus	12.53	kJ/mol	Joback Method
hvap	53.83	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.753		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	1052.00		NIST Webbook
tb	504.73	K	Joback Method
tc	681.69	K	Joback Method
tf	249.40	K	Joback Method
vc	0.441	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.07	J/molxK	504.73	Joback Method
cpg	276.55	J/molxK	534.22	Joback Method
cpg	286.57	J/molxK	563.72	Joback Method
cpg	296.15	J/molxK	593.21	Joback Method
cpg	305.30	J/molxK	622.70	Joback Method
cpg	314.03	J/molxK	652.20	Joback Method
cpg	322.35	J/molxK	681.69	Joback Method
dvisc	0.0707125	Paxs	249.40	Joback Method
dvisc	0.0121690	Paxs	291.95	Joback Method

dvisc	0.0032769	Paxs	334.51	Joback Method
dvisc	0.0011865	Paxs	377.06	Joback Method
dvisc	0.0005279	Paxs	419.62	Joback Method
dvisc	0.0002727	Paxs	462.18	Joback Method
dvisc	0.0001574	Paxs	504.73	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=R503496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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