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
CAS: 3302-06-5

Physical Properties

Property code	Value	Unit	Source
hf	-558.19	kJ/mol	Cheméo Relay (1.0)
hfus	12.53	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Cheméo Relay (1.0)
ie	10.07	eV	Cheméo Relay (1.0)
log10ws	-1.43		Cheméo Relay (1.0)
logp	1.753		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
tb	467.71	K	Cheméo Relay (1.0)
tc	651.17	K	Cheméo Relay (1.0)
tf	278.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.07	J/mol×K	504.73	Joback Method
cpg	276.55	J/mol×K	534.22	Joback Method
cpg	286.57	J/mol×K	563.72	Joback Method
cpg	296.15	J/mol×K	593.21	Joback Method
cpg	305.30	J/mol×K	622.70	Joback Method
cpg	314.03	J/mol×K	652.20	Joback Method
cpg	322.35	J/mol×K	681.69	Joback Method
dvisc	0.0707125	Pa×s	249.40	Joback Method
dvisc	0.0121690	Pa×s	291.95	Joback Method
dvisc	0.0032769	Pa×s	334.51	Joback Method

dvisc	0.0011865	Pa×s	377.06	Joback Method
dvisc	0.0005279	Pa×s	419.62	Joback Method
dvisc	0.0002727	Pa×s	462.18	Joback Method
dvisc	0.0001574	Pa×s	504.73	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3302065&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point