

2-Isopropyl-5-oxo-hexanoic acid

Inchi:	InChI=1S/C9H16O3/c1-6(2)8(9(11)12)5-4-7(3)10/h6,8H,4-5H2,1-3H3,(H,11,12)
InchiKey:	GBNBHMJSMSODSZ-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	CC(=O)CCC(C(=O)O)C(C)C
Mol. weight [g/mol]:	172.22

Physical Properties

Property code	Value	Unit	Source
gf	-374.64	kJ/mol	Joback Method
hf	-617.04	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	65.02	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.712		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
ripol	2570.00		NIST Webbook
tb	604.36	K	Joback Method
tc	786.29	K	Joback Method
tf	321.87	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.45	J/molxK	604.36	Joback Method
cpg	384.73	J/molxK	634.68	Joback Method
cpg	395.46	J/molxK	665.00	Joback Method
cpg	405.65	J/molxK	695.32	Joback Method
cpg	415.32	J/molxK	725.64	Joback Method
cpg	424.48	J/molxK	755.97	Joback Method
cpg	433.14	J/molxK	786.29	Joback Method
dvisc	0.0137516	Paxs	321.87	Joback Method
dvisc	0.0035083	Paxs	368.95	Joback Method

dvisc	0.0012193	Paxs	416.03	Joback Method
dvisc	0.0005254	Paxs	463.12	Joback Method
dvisc	0.0002644	Paxs	510.20	Joback Method
dvisc	0.0001495	Paxs	557.28	Joback Method
dvisc	0.0000923	Paxs	604.36	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=R326135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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