

2-Isopropyl-5-methyl-hexanoic acid

Inchi:	InChI=1S/C10H20O2/c1-7(2)5-6-9(8(3)4)10(11)12/h7-9H,5-6H2,1-4H3,(H,11,12)
InchiKey:	ZOINHQMIOAPOSQ-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CC(C)CCC(C(=O)O)C(C)C
Mol. weight [g/mol]:	172.26
CAS:	4384-07-0

Physical Properties

Property code	Value	Unit	Source
gf	-239.74	kJ/mol	Joback Method
hf	-530.38	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	60.11	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.779		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
ripol	2034.00		NIST Webbook
ripol	2034.00		NIST Webbook
tb	572.93	K	Joback Method
tc	748.66	K	Joback Method
tf	268.21	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.87	J/mol×K	572.93	Joback Method
cpg	417.12	J/mol×K	602.22	Joback Method
cpg	429.76	J/mol×K	631.51	Joback Method
cpg	441.83	J/mol×K	660.79	Joback Method
cpg	453.33	J/mol×K	690.08	Joback Method
cpg	464.28	J/mol×K	719.37	Joback Method
cpg	474.69	J/mol×K	748.66	Joback Method

dvisc	0.0637662	Paxs	268.21	Joback Method
dvisc	0.0088269	Paxs	319.00	Joback Method
dvisc	0.0021034	Paxs	369.78	Joback Method
dvisc	0.0007087	Paxs	420.57	Joback Method
dvisc	0.0003019	Paxs	471.36	Joback Method
dvisc	0.0001518	Paxs	522.14	Joback Method
dvisc	0.0000862	Paxs	572.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4384070&Units=SI

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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