

2,6-Dimethyl-heptanoic acid

Inchi:	InChI=1S/C9H18O2/c1-7(2)5-4-6-8(3)9(10)11/h7-8H,4-6H2,1-3H3,(H,10,11)
InchiKey:	MDAPKSVKYITQHQ-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CC(C)CCCC(C)C(=O)O
Mol. weight [g/mol]:	158.24

Physical Properties

Property code	Value	Unit	Source
gf	-245.72	kJ/mol	Joback Method
hf	-504.46	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	58.28	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.533		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
ripol	2012.00		NIST Webbook
ripol	2012.00		NIST Webbook
tb	550.49	K	Joback Method
tc	724.45	K	Joback Method
tf	271.94	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.90	J/molxK	550.49	Joback Method
cpg	368.12	J/molxK	579.48	Joback Method
cpg	379.81	J/molxK	608.48	Joback Method
cpg	390.98	J/molxK	637.47	Joback Method
cpg	401.64	J/molxK	666.46	Joback Method
cpg	411.80	J/molxK	695.45	Joback Method
cpg	421.50	J/molxK	724.45	Joback Method
dvisc	0.0424192	Paxs	271.94	Joback Method

dvisc	0.0076296	Paxs	318.37	Joback Method
dvisc	0.0021236	Paxs	364.79	Joback Method
dvisc	0.0007890	Paxs	411.22	Joback Method
dvisc	0.0003583	Paxs	457.64	Joback Method
dvisc	0.0001882	Paxs	504.07	Joback Method
dvisc	0.0001102	Paxs	550.49	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=R326115&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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