

3,3-Dimethylheptanoic acid

Inchi:	InChI=1S/C9H18O2/c1-4-5-6-9(2,3)7-8(10)11/h4-7H2,1-3H3,(H,10,11)
InchiKey:	KLRHFTOZNSFIHY-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCC(C)(C)CC(=O)O
Mol. weight [g/mol]:	158.24
CAS:	67061-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-238.00	kJ/mol	Joback Method
hf	-502.65	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.678		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	491.00 ± 2.00	K	NIST Webbook
tc	724.68	K	Joback Method
tf	304.36	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.58	J/molxK	548.14	Joback Method
cpg	414.44	J/molxK	695.26	Joback Method
cpg	404.40	J/molxK	665.83	Joback Method
cpg	393.82	J/molxK	636.41	Joback Method
cpg	382.67	J/molxK	606.99	Joback Method
cpg	370.94	J/molxK	577.56	Joback Method
cpg	423.96	J/molxK	724.68	Joback Method
dvisc	0.0001170	Paxs	548.14	Joback Method
dvisc	0.0001912	Paxs	507.51	Joback Method

dvisc	0.0003405	Paxs	466.88	Joback Method
dvisc	0.0006767	Paxs	426.25	Joback Method
dvisc	0.0015543	Paxs	385.62	Joback Method
dvisc	0.0043425	Paxs	344.99	Joback Method
dvisc	0.0159623	Paxs	304.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67061307&Units=SI
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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