

3,7-Dimethyl-octanoic acid

Inchi:	InChI=1S/C10H20O2/c1-8(2)5-4-6-9(3)7-10(11)12/h8-9H,4-7H2,1-3H3,(H,11,12)
InchiKey:	DGGBNSXAFVNQJU-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CC(C)CCCC(C)CC(=O)O
Mol. weight [g/mol]:	172.26
CAS:	5698-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-237.30	kJ/mol	Joback Method
hf	-525.10	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	60.50	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.924		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1359.00		NIST Webbook
tb	573.37	K	Joback Method
tc	746.05	K	Joback Method
tf	283.21	K	Joback Method
vc	0.609	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.51	J/molxK	573.37	Joback Method
cpg	416.47	J/molxK	602.15	Joback Method
cpg	428.87	J/molxK	630.93	Joback Method
cpg	440.70	J/molxK	659.71	Joback Method
cpg	452.00	J/molxK	688.49	Joback Method
cpg	462.78	J/molxK	717.27	Joback Method
cpg	473.04	J/molxK	746.05	Joback Method
dvisc	0.0330442	Paxs	283.21	Joback Method

dvisc	0.0060601	Paxs	331.57	Joback Method
dvisc	0.0017116	Paxs	379.93	Joback Method
dvisc	0.0006431	Paxs	428.29	Joback Method
dvisc	0.0002948	Paxs	476.65	Joback Method
dvisc	0.0001560	Paxs	525.01	Joback Method
dvisc	0.0000919	Paxs	573.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5698271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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