

4-Pentenoic acid, 2,2-dimethyl-

Inchi:	InChI=1S/C7H12O2/c1-4-5-7(2,3)6(8)9/h4H,1,5H2,2-3H3,(H,8,9)
InchiKey:	BGUAPYRHJPWVEM-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CCC(C)(C)C(=O)O
Mol. weight [g/mol]:	128.17
CAS:	16386-93-9

Physical Properties

Property code	Value	Unit	Source
gf	-167.00	kJ/mol	Joback Method
hf	-335.94	kJ/mol	Joback Method
hfus	10.88	kJ/mol	Joback Method
hvap	52.64	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.673		Crippen Method
mvol	112.630	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	499.06	K	Joback Method
tc	682.42	K	Joback Method
tf	280.06	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.13	J/molxK	499.06	Joback Method
cpg	261.21	J/molxK	529.62	Joback Method
cpg	270.72	J/molxK	560.18	Joback Method
cpg	279.68	J/molxK	590.74	Joback Method
cpg	288.13	J/molxK	621.30	Joback Method
cpg	296.09	J/molxK	651.86	Joback Method
cpg	303.60	J/molxK	682.42	Joback Method
dvisc	0.0233000	Paxs	280.06	Joback Method
dvisc	0.0064738	Paxs	316.56	Joback Method

dvisc	0.0023440	Paxs	353.06	Joback Method
dvisc	0.0010267	Paxs	389.56	Joback Method
dvisc	0.0005180	Paxs	426.06	Joback Method
dvisc	0.0002912	Paxs	462.56	Joback Method
dvisc	0.0001780	Paxs	499.06	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	2.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16386939&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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