

Hexanedioic acid, 2-methyl-

Inchi:	InChI=1S/C7H12O4/c1-5(7(10)11)3-2-4-6(8)9/h5H,2-4H2,1H3,(H,8,9)(H,10,11)
InchiKey:	JZUMVFMLJGSMRF-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CC(CCCC(=O)O)C(=O)O
Mol. weight [g/mol]:	160.17
CAS:	626-70-0

Physical Properties

Property code	Value	Unit	Source
gf	-525.86	kJ/mol	Joback Method
hf	-722.71	kJ/mol	Joback Method
hfus	21.74	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.962		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	651.22	K	Joback Method
tc	826.91	K	Joback Method
tf	336.00 ± 4.00	K	NIST Webbook
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.86	J/molxK	651.22	Joback Method
cpg	332.86	J/molxK	680.50	Joback Method
cpg	340.46	J/molxK	709.78	Joback Method
cpg	347.66	J/molxK	739.07	Joback Method
cpg	354.49	J/molxK	768.35	Joback Method
cpg	360.95	J/molxK	797.63	Joback Method
cpg	367.05	J/molxK	826.91	Joback Method
dvisc	0.0074203	Paxs	375.15	Joback Method
dvisc	0.0017611	Paxs	421.16	Joback Method

dvisc	0.0005549	Paxs	467.17	Joback Method
dvisc	0.0002150	Paxs	513.19	Joback Method
dvisc	0.0000974	Paxs	559.20	Joback Method
dvisc	0.0000498	Paxs	605.21	Joback Method
dvisc	0.0000280	Paxs	651.22	Joback Method

Sources

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=C626700&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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