

3-Hexenedioic acid, trans-

Inchi:	InChI=1S/C6H8O4/c7-5(8)3-1-2-4-6(9)10/h1-2H,3-4H2,(H,7,8)(H,9,10)/b2-1+
InchiKey:	YHGNXQAFNHCBTK-OWOJBTEDSA-N
Formula:	C6H8O4
SMILES:	O=C(O)CC=CCC(=O)O
Mol. weight [g/mol]:	144.13
CAS:	29311-53-3

Physical Properties

Property code	Value	Unit	Source
gf	-451.62	kJ/mol	Joback Method
hf	-579.57	kJ/mol	Joback Method
hfus	22.87	kJ/mol	Joback Method
hvap	75.76	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.492		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
tb	632.94	K	Joback Method
tc	812.61	K	Joback Method
tf	373.80	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.48	J/molxK	632.94	Joback Method
cpg	261.84	J/molxK	662.88	Joback Method
cpg	267.85	J/molxK	692.83	Joback Method
cpg	273.53	J/molxK	722.77	Joback Method
cpg	278.90	J/molxK	752.72	Joback Method
cpg	283.98	J/molxK	782.66	Joback Method
cpg	288.78	J/molxK	812.61	Joback Method
dvisc	0.0059097	Paxs	373.80	Joback Method
dvisc	0.0015702	Paxs	416.99	Joback Method

dvisc	0.0005351	Paxs	460.18	Joback Method
dvisc	0.0002193	Paxs	503.37	Joback Method
dvisc	0.0001035	Paxs	546.56	Joback Method
dvisc	0.0000545	Paxs	589.75	Joback Method
dvisc	0.0000314	Paxs	632.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C29311533&Units=SI

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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