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/mol×K	632.94	Joback Method
cpg	261.84	J/mol×K	662.88	Joback Method
cpg	267.85	J/mol×K	692.83	Joback Method
cpg	273.53	J/mol×K	722.77	Joback Method
cpg	278.90	J/mol×K	752.72	Joback Method
cpg	283.98	J/mol×K	782.66	Joback Method
cpg	288.78	J/mol×K	812.61	Joback Method
dvisc	0.0059097	Pa×s	373.80	Joback Method
dvisc	0.0015702	Pa×s	416.99	Joback Method

dvisc	0.0005351	Pa×s	460.18	Joback Method
dvisc	0.0002193	Pa×s	503.37	Joback Method
dvisc	0.0001035	Pa×s	546.56	Joback Method
dvisc	0.0000545	Pa×s	589.75	Joback Method
dvisc	0.0000314	Pa×s	632.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29311533&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume