

3-Hydroxy-3-methyl-2,4-nonanedione

Inchi:	InChI=1S/C10H18O3/c1-4-5-6-7-9(12)10(3,13)8(2)11/h13H,4-7H2,1-3H3
InchiKey:	LWAGDIOTWITDPB-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CCCCC(=O)C(C)(O)C(C)=O
Mol. weight [g/mol]:	186.25

Physical Properties

Property code	Value	Unit	Source
gf	-358.50	kJ/mol	Joback Method
hf	-635.87	kJ/mol	Joback Method
hfus	21.53	kJ/mol	Joback Method
hvap	66.73	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.476		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinqol	1202.00		NIST Webbook
tb	624.89	K	Joback Method
tc	807.74	K	Joback Method
tf	365.56	K	Joback Method
vc	0.616	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.60	J/molxK	624.89	Joback Method
cpg	436.53	J/molxK	655.37	Joback Method
cpg	447.81	J/molxK	685.84	Joback Method
cpg	458.48	J/molxK	716.32	Joback Method
cpg	468.56	J/molxK	746.79	Joback Method
cpg	478.08	J/molxK	777.27	Joback Method
cpg	487.06	J/molxK	807.74	Joback Method
dvisc	0.0052791	Paxs	365.56	Joback Method
dvisc	0.0018081	Paxs	408.78	Joback Method

dvisc	0.0007601	Paxs	452.00	Joback Method
dvisc	0.0003717	Paxs	495.23	Joback Method
dvisc	0.0002039	Paxs	538.45	Joback Method
dvisc	0.0001223	Paxs	581.67	Joback Method
dvisc	0.0000787	Paxs	624.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587236&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
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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