3,3-Dimethyl-2,7-octanedione

Inchi: InChI=1S/C10H18O2/c1-8(11)6-5-7-10(3,4)9(2)12/h5-7H2,1-4H3
InchiKey: RMVQEJVZIPNRJR-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(=O)CCCC(C)(C)C(C)=O
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-221.68	kJ/mol	Joback Method
hf	-483.64	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	50.05	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.361		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1290.00		NIST Webbook
tb	532.71	K	Joback Method
tc	725.16	K	Joback Method
tf	304.74	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.04	J/mol×K	532.71	Joback Method
cpg	432.90	J/mol×K	693.09	Joback Method
cpg	421.37	J/mol×K	661.01	Joback Method
cpg	409.15	J/mol×K	628.94	Joback Method
cpg	396.21	J/mol×K	596.86	Joback Method
cpg	382.51	J/mol×K	564.79	Joback Method
cpg	443.78	J/mol×K	725.16	Joback Method
dvisc	0.0002734	Pa×s	532.71	Joback Method
dvisc	0.0003640	Pa×s	494.72	Joback Method

dvisc	0.0005082	Pa×s	456.72	Joback Method
dvisc	0.0007539	Pa×s	418.73	Joback Method
dvisc	0.0012100	Pa×s	380.73	Joback Method
dvisc	0.0021567	Pa×s	342.74	Joback Method
dvisc	0.0044400	Pa×s	304.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R439553&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