2,7-Octanedione, 4,4,5,5-tetramethyl-

Other names: 4,4,5,5-Tetramethyl-2,7-octanedione
Inchi: InChI=1S/C12H22O2/c1-9(13)7-11(3,4)12(5,6)8-10(2)14/h7-8H2,1-6H3
InchiKey: GTRYXHORFPEEMD-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CC(=O)CC(C)(C)C(C)(C)CC(C)=O
Mol. weight [g/mol]: 198.30
CAS: 17663-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-202.00	kJ/mol	Joback Method
hf	-533.67	kJ/mol	Joback Method
hfus	15.21	kJ/mol	Joback Method
hvap	53.21	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.997		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
tb	575.24	K	Joback Method
tc	773.66	K	Joback Method
tf	329.70	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.82	J/mol×K	575.24	Joback Method
cpg	484.46	J/mol×K	608.31	Joback Method
cpg	500.07	J/mol×K	641.38	Joback Method
cpg	514.73	J/mol×K	674.45	Joback Method
cpg	528.48	J/mol×K	707.52	Joback Method
cpg	541.38	J/mol×K	740.59	Joback Method
cpg	553.48	J/mol×K	773.66	Joback Method
dvisc	0.0045669	Pa×s	329.70	Joback Method

dvisc	0.0020349	Pa×s	370.62	Joback Method
dvisc	0.0010648	Pa×s	411.55	Joback Method
dvisc	0.0006265	Pa×s	452.47	Joback Method
dvisc	0.0004025	Pa×s	493.39	Joback Method
dvisc	0.0002767	Pa×s	534.32	Joback Method
dvisc	0.0002006	Pa×s	575.24	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=C17663273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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