

1,1,2,2-Tetraacetyethane

Other names:	3,4-Diacetyl-2,5-hexanedione tetra Acetyl ethane 2,5-Hexanedione, 3,4-diacetyl- 3.3'-Bis(acetylacetone) 3,4-diacetylhexane-2,5-dione
Inchi:	InChI=1S/C10H14O4/c1-5(11)9(6(2)12)10(7(3)13)8(4)14/h9-10H,1-4H3
InchiKey:	CSKRBHOAJUMOKJ-UHFFFAOYSA-N
Formula:	C10H14O4
SMILES:	CC(=O)C(C(C)=O)C(C(C)=O)C(C)=O
Mol. weight [g/mol]:	198.22
CAS:	5027-32-7

Physical Properties

Property code	Value	Unit	Source
gf	-487.24	kJ/mol	Joback Method
hf	-710.61	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.575		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	642.80	K	Joback Method
tc	847.37	K	Joback Method
tf	372.18	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.70	J/molxK	642.80	Joback Method
cpg	453.32	J/molxK	813.28	Joback Method
cpg	444.16	J/molxK	779.18	Joback Method
cpg	434.34	J/molxK	745.09	Joback Method

cpg	423.83	J/molxK	710.99	Joback Method
cpg	412.62	J/molxK	676.90	Joback Method
cpg	461.83	J/molxK	847.37	Joback Method
dvisc	0.0002700	Paxs	642.80	Joback Method
dvisc	0.0003542	Paxs	597.70	Joback Method
dvisc	0.0004857	Paxs	552.59	Joback Method
dvisc	0.0007045	Paxs	507.49	Joback Method
dvisc	0.0010988	Paxs	462.39	Joback Method
dvisc	0.0018866	Paxs	417.28	Joback Method
dvisc	0.0036927	Paxs	372.18	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=C5027327&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

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