sym-Tetraacetylethane

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

Physical Properties

Property code	Value	Unit	Source
af	0.5252		Cheméo Relay (1.0)
gf	-487.24	kJ/mol	Joback Method
hf	-733.57	kJ/mol	Cheméo Relay (1.0)
hfus	21.01	kJ/mol	Joback Method
hvap	69.38	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-0.95		Cheméo Relay (1.0)
logp	0.575		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	505.76	K	Cheméo Relay (1.0)
tc	710.88	K	Cheméo Relay (1.0)
tf	375.60	K	Cheméo Relay (1.0)
vc	0.527	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.70	J/mol×K	642.80	Joback Method
cpg	412.62	J/mol×K	676.90	Joback Method
cpg	423.83	J/mol×K	710.99	Joback Method

cpg	434.34	J/mol×K	745.09	Joback Method
cpg	444.16	J/mol×K	779.18	Joback Method
cpg	453.32	J/mol×K	813.28	Joback Method
cpg	461.83	J/mol×K	847.37	Joback Method
dvisc	0.0036927	Pa×s	372.18	Joback Method
dvisc	0.0018866	Pa×s	417.28	Joback Method
dvisc	0.0010988	Pa×s	462.39	Joback Method
dvisc	0.0007045	Pa×s	507.49	Joback Method
dvisc	0.0004857	Pa×s	552.59	Joback Method
dvisc	0.0003542	Pa×s	597.70	Joback Method
dvisc	0.0002700	Pa×s	642.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5027327&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
ie: Ionization energy
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