

acetyl ethaneperoxoate

Inchi:	InChI=1S/C4H6O4/c1-3(5)7-8-4(2)6/h1-2H3
InchiKey:	ZQMIGQNCOMNODD-UHFFFAOYSA-N
Formula:	C4H6O4
SMILES:	CC(=O)OOC(C)=O
Mol. weight [g/mol]:	118.09
CAS:	110-22-5

Physical Properties

Property code	Value	Unit	Source
af	0.5577		Cheméo Relay (1.0)
gf	-637.94	kJ/mol	Joback Method
hf	-565.89	kJ/mol	Cheméo Relay (1.0)
hfus	14.85	kJ/mol	Joback Method
hvap	58.23	kJ/mol	Cheméo Relay (1.0)
ie	9.87	eV	Cheméo Relay (1.0)
log10ws	-0.61		Cheméo Relay (1.0)
logp	0.028		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	417.52	K	Cheméo Relay (1.0)
tc	578.03	K	Cheméo Relay (1.0)
tf	303.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.326	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	5.00700e+01
Coeff. B	2.74240e-01

Coeff. C	-4.60000e-06
Coeff. D	-7.78000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.18006e+01
Coeff. B	1.46652e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	303.15
Temperature range (K), max.	414.32

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvac:	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

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