1,5-Diacetoxypentane

Other names: 1,5-Pentanediol diacetate
Pentamethylene acetate
pentane-1,5-diyl diacetate
Inchi: InChI=1S/C9H16O4/c1-8(10)12-6-4-3-5-7-13-9(2)11/h3-7H2,1-2H3
InchiKey: PIJBVCVBCQOWMM-UHFFFAOYSA-N
Formula: C9H16O4
SMILES: CC(=O)OCCCCCOC(C)=O
Mol. weight [g/mol]: 188.22
CAS: 6963-44-6

Physical Properties

Property code	Value	Unit	Source
gf	-442.94	kJ/mol	Joback Method
hf	-718.69	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	53.94	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.283		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
tb	517.00	K	NIST Webbook
tc	739.72	K	Joback Method
tf	335.51	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.05	J/mol×K	557.90	Joback Method
cpg	380.43	J/mol×K	588.20	Joback Method
cpg	392.33	J/mol×K	618.51	Joback Method
cpg	403.74	J/mol×K	648.81	Joback Method
cpg	414.66	J/mol×K	679.11	Joback Method
cpg	425.08	J/mol×K	709.42	Joback Method

cpg	435.00	J/mol×K	739.72	Joback Method
dvisc	0.0019834	Pa×s	335.51	Joback Method
dvisc	0.0011310	Pa×s	372.57	Joback Method
dvisc	0.0007139	Pa×s	409.64	Joback Method
dvisc	0.0004864	Pa×s	446.70	Joback Method
dvisc	0.0003515	Pa×s	483.77	Joback Method
dvisc	0.0002660	Pa×s	520.84	Joback Method
dvisc	0.0002089	Pa×s	557.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.70	K	0.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6963446&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

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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume