1,3-Propanediol, diacetate

Other names:	Trimethylene acetate
	1,3-Diacetoxypropane
	1,3-Propylene diacetate
	1,3-Propylene glycol diacetate
	Diacetate of 1,3-propanediol
Inchi:	InChI=1S/C7H12O4/c1-6(8)10-4-3-5-11-7(2)9/h3-5H2,1-2H3
InchiKey:	DSVGICPKBRQDDX-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CC(=O)OCCCOC(C)=O
Mol. weight [g/mol]:	160.17
CAS:	628-66-0

Physical Properties

Property code	Value	Unit	Source
gf	-459.78	kJ/mol	Joback Method
hf	-677.41	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	49.49	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.503		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1089.00		NIST Webbook
rinpol	1089.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	482.50 ± 0.50	K	NIST Webbook
tb	482.70	K	NIST Webbook
tc	697.87	K	Joback Method
tf	312.97	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.30	J/mol×K	512.14	Joback Method
cpg	326.76	J/mol×K	666.91	Joback Method
cpg	317.83	J/mol×K	635.96	Joback Method
cpg	308.51	J/mol×K	605.00	Joback Method
cpg	298.81	J/mol×K	574.05	Joback Method
cpg	288.74	J/mol×K	543.09	Joback Method
cpg	335.29	J/mol×K	697.87	Joback Method
dvisc	0.0002482	Pa×s	512.14	Joback Method
dvisc	0.0003126	Pa×s	478.94	Joback Method
dvisc	0.0004076	Pa×s	445.75	Joback Method
dvisc	0.0005546	Pa×s	412.56	Joback Method
dvisc	0.0007964	Pa×s	379.36	Joback Method
dvisc	0.0012258	Pa×s	346.17	Joback Method
dvisc	0.0020676	Pa×s	312.97	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628660&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume