1,2-Propanediol, diacetate

Other names:	1,2-Diacetoxypropane
	Methylethylene acetate
	Methylethylene diacetate
	Propylene acetate
	Propylene diacetate
	1,2-Propylene diacetate
	Propylene glycol diacetate
	«alpha»-Propylene glycol diacetate
	1,2-Propylene glycol diacetate
	Propane-1,2-diol diacetate
	1,2-Propanediol, 1,2-diacetate
	NSC 75843
	2-(Acetyloxy)-1-methylethyl acetate
	propane-1,2-diyl diacetate
Inchi:	InChI=1S/C7H12O4/c1-5(11-7(3)9)4-10-6(2)8/h5H,4H2,1-3H3
InchiKey:	MLHOXUWWKVQEJB-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CC(=O)OCC(C)OC(C)=O
Mol. weight [g/mol]:	160.17
CAS:	623-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-462.22	kJ/mol	Joback Method
hf	-682.69	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.501		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	999.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	996.00		NIST Webbook

rinpol	1000.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1018.50		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	996.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1496.00		NIST Webbook
tb	463.70	K	NIST Webbook
tc	701.34	K	Joback Method
tf	297.97	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.95	J/mol×K	701.34	Joback Method
cpg	278.59	J/mol×K	511.70	Joback Method
cpg	289.32	J/mol×K	543.31	Joback Method
cpg	299.65	J/mol×K	574.91	Joback Method
cpg	309.59	J/mol×K	606.52	Joback Method
cpg	319.13	J/mol×K	638.13	Joback Method
cpg	328.25	J/mol×K	669.73	Joback Method
dvisc	0.0002344	Pa×s	511.70	Joback Method
dvisc	0.0027013	Pa×s	297.97	Joback Method
dvisc	0.0014459	Pa×s	333.59	Joback Method
dvisc	0.0008732	Pa×s	369.21	Joback Method
dvisc	0.0005762	Pa×s	404.84	Joback Method
dvisc	0.0004067	Pa×s	440.46	Joback Method
dvisc	0.0003024	Pa×s	476.08	Joback Method
hvapt	54.90	kJ/mol	342.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.50 ± 0.50	K	2.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623847&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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume