

2,2,4-Trimethyl-1,3-pentenediol diacetate

Inchi:	InChI=1S/C12H22O4/c1-8(2)11(16-10(4)14)12(5,6)7-15-9(3)13/h8,11H,7H2,1-6H3
InchiKey:	AVQIDJASTVSUMQ-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CC(=O)OCC(C)(C)C(OC(C)=O)C(C)C
Mol. weight [g/mol]:	230.30
CAS:	4100-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-419.72	kJ/mol	Joback Method
hf	-799.92	kJ/mol	Joback Method
hfus	17.95	kJ/mol	Joback Method
hvap	58.55	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.163		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
tb	622.43	K	Joback Method
tc	814.75	K	Joback Method
tf	341.74	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.80	J/molxK	622.43	Joback Method
cpg	590.42	J/molxK	782.70	Joback Method
cpg	577.89	J/molxK	750.64	Joback Method
cpg	564.57	J/molxK	718.59	Joback Method
cpg	550.46	J/molxK	686.54	Joback Method
cpg	535.54	J/molxK	654.48	Joback Method
cpg	602.20	J/molxK	814.75	Joback Method
dvisc	0.0001161	Paxs	622.43	Joback Method
dvisc	0.0001608	Paxs	575.65	Joback Method

dvisc	0.0002358	Paxs	528.87	Joback Method
dvisc	0.0003726	Paxs	482.09	Joback Method
dvisc	0.0006495	Paxs	435.30	Joback Method
dvisc	0.0012944	Paxs	388.52	Joback Method
dvisc	0.0031157	Paxs	341.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4100098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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