

threitol, acetylated

Inchi:	InChI=1S/C12H18O8/c1-7(13)17-5-11(19-9(3)15)12(20-10(4)16)6-18-8(2)14/h11-12H,5-6
InchiKey:	RSZROFFHBBZJAD-RYUDHWBXSA-N
Formula:	C12H18O8
SMILES:	CC(=O)OCC(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]:	290.27

Physical Properties

Property code	Value	Unit	Source
gf	-890.40	kJ/mol	Joback Method
hf	-1280.77	kJ/mol	Joback Method
hfus	30.94	kJ/mol	Joback Method
hvap	78.15	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	-0.024		Crippen Method
mcvol	209.700	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1580.80		NIST Webbook
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tb	778.24	K	Joback Method
tc	974.96	K	Joback Method
tf	483.64	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.12	J/molxK	778.24	Joback Method
cpg	657.35	J/molxK	942.17	Joback Method
cpg	649.02	J/molxK	909.39	Joback Method
cpg	639.70	J/molxK	876.60	Joback Method
cpg	629.43	J/molxK	843.81	Joback Method
cpg	618.23	J/molxK	811.03	Joback Method
cpg	664.67	J/molxK	974.96	Joback Method
dvisc	0.0000723	Paxs	778.24	Joback Method

dvisc	0.0000937	Paxs	729.14	Joback Method
dvisc	0.0001259	Paxs	680.04	Joback Method
dvisc	0.0001773	Paxs	630.94	Joback Method
dvisc	0.0002645	Paxs	581.84	Joback Method
dvisc	0.0004246	Paxs	532.74	Joback Method
dvisc	0.0007505	Paxs	483.64	Joback Method

Sources

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=R489068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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