1,3,5-Trioxane, 2,4,6-tris(1-methylethyl)-

Other names:	s-Trioxane, 2,4,6-triisopropyl-
	Sunsubly B
	Triisopropyl-s-trioxane
	1,3,5-Trioxane, 2,4,6-triisopropyl-
	2,4,6-Triisopropyl-1,3,5-trioxane
	2,4,6-Triisopropyltrioxane
	2,4,6-Tri-isopropyl-[1,3,5]trioxane, stereoisomer 2
Inchi:	InChI=1S/C12H24O3/c1-7(2)10-13-11(8(3)4)15-12(14-10)9(5)6/h7-12H,1-6H3
InchiKey:	XYIANCZIPATGDH-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	CC(C)C1OC(C(C)C)OC(C(C)C)O1
Mol. weight [g/mol]:	216.32
CAS:	7580-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-206.49	kJ/mol	Joback Method
hf	-689.21	kJ/mol	Joback Method
hfus	34.18	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.996		Crippen Method
mcvol	186.690	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
ripol	1230.00		NIST Webbook
tb	563.70	K	Joback Method
tc	764.97	K	Joback Method
tf	258.61	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.90	J/mol×K	563.70	Joback Method

cpg	597.76	J/mol×K	731.43	Joback Method
cpg	581.03	J/mol×K	697.88	Joback Method
cpg	563.29	J/mol×K	664.34	Joback Method
cpg	544.53	J/mol×K	630.79	Joback Method
cpg	524.74	J/mol×K	597.25	Joback Method
cpg	613.50	J/mol×K	764.97	Joback Method
dvisc	0.0002297	Pa×s	563.70	Joback Method
dvisc	0.0003188	Pa×s	512.85	Joback Method
dvisc	0.0004755	Pa×s	462.00	Joback Method
dvisc	0.0007830	Pa×s	411.16	Joback Method
dvisc	0.0014844	Pa×s	360.31	Joback Method
dvisc	0.0034721	Pa×s	309.46	Joback Method
dvisc	0.0113436	Pa×s	258.61	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7580123&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume