

2,4,6-Tri-isopropyl-[1,3,5]trioxane, stereoisomer 1

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

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	1160.00		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/molxK	563.70	Joback Method
cpg	524.74	J/molxK	597.25	Joback Method
cpg	544.53	J/molxK	630.79	Joback Method
cpg	563.29	J/molxK	664.34	Joback Method
cpg	581.03	J/molxK	697.88	Joback Method
cpg	597.76	J/molxK	731.43	Joback Method
cpg	613.50	J/molxK	764.97	Joback Method
dvisc	0.0113436	Paxs	258.61	Joback Method
dvisc	0.0034721	Paxs	309.46	Joback Method

dvisc	0.0014844	Paxs	360.31	Joback Method
dvisc	0.0007830	Paxs	411.16	Joback Method
dvisc	0.0004755	Paxs	462.00	Joback Method
dvisc	0.0003188	Paxs	512.85	Joback Method
dvisc	0.0002297	Paxs	563.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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