

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

Inchi:	InChI=1S/C15H30O3/c1-10(2)7-13-16-14(8-11(3)4)18-15(17-13)9-12(5)6/h10-15H,7-9H2
InchiKey:	SBVHSWJZXOYLFE-UHFFFAOYSA-N
Formula:	C15H30O3
SMILES:	CC(C)CC1OC(CC(C)C)OC(CC(C)C)O1
Mol. weight [g/mol]:	258.40

Physical Properties

Property code	Value	Unit	Source
gf	-181.23	kJ/mol	Joback Method
hf	-751.13	kJ/mol	Joback Method
hfus	41.95	kJ/mol	Joback Method
hvap	61.16	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.166		Crippen Method
mcvol	228.960	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
ripol	1410.00		NIST Webbook
tb	632.34	K	Joback Method
tc	825.80	K	Joback Method
tf	292.42	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.68	J/molxK	632.34	Joback Method
cpg	688.50	J/molxK	664.58	Joback Method
cpg	709.19	J/molxK	696.83	Joback Method
cpg	728.76	J/molxK	729.07	Joback Method
cpg	747.24	J/molxK	761.31	Joback Method
cpg	764.64	J/molxK	793.56	Joback Method
cpg	780.98	J/molxK	825.80	Joback Method
dvisc	0.0085194	Paxs	292.42	Joback Method
dvisc	0.0025893	Paxs	349.07	Joback Method

dvisc	0.0010975	Paxs	405.73	Joback Method
dvisc	0.0005741	Paxs	462.38	Joback Method
dvisc	0.0003459	Paxs	519.03	Joback Method
dvisc	0.0002303	Paxs	575.69	Joback Method
dvisc	0.0001649	Paxs	632.34	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495048&Units=SI

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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