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

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	1450.00		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/mol×K	632.34	Joback Method
cpg	688.50	J/mol×K	664.58	Joback Method
cpg	709.19	J/mol×K	696.83	Joback Method
cpg	728.76	J/mol×K	729.07	Joback Method
cpg	747.24	J/mol×K	761.31	Joback Method
cpg	764.64	J/mol×K	793.56	Joback Method
cpg	780.98	J/mol×K	825.80	Joback Method
dvisc	0.0085194	Pa×s	292.42	Joback Method
dvisc	0.0025893	Pa×s	349.07	Joback Method

dvisc	0.0010975	Pa×s	405.73	Joback Method
dvisc	0.0005741	Pa×s	462.38	Joback Method
dvisc	0.0003459	Pa×s	519.03	Joback Method
dvisc	0.0002303	Pa×s	575.69	Joback Method
dvisc	0.0001649	Pa×s	632.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495053&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