cis-2,4,6-Trimethyl-1,3,5-trioxane

Inchi: InChI=1S/C6H12O3/c1-4-7-5(2)9-6(3)8-4/h4-6H,1-3H3/t4-,5+,6-
InchiKey: SQYNKIJPMDEDEG-FPFOFBBKSA-N
Formula: C6H12O3
SMILES: CC1OC(C)OC(C)O1
Mol. weight [g/mol]: 132.16
CAS: 1499-02-1

Physical Properties

Property code	Value	Unit	Source
chl	-3394.20 ± 2.60	kJ/mol	NIST Webbook
gf	-249.69	kJ/mol	Joback Method
hf	-636.20 ± 3.00	kJ/mol	NIST Webbook
hfl	-681.80 ± 2.60	kJ/mol	NIST Webbook
hfus	29.21	kJ/mol	Joback Method
hvap	45.60	kJ/mol	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.088		Crippen Method
mcvol	102.150	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	427.74	K	Joback Method
tc	632.02	K	Joback Method
tf	235.99	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.56	J/mol×K	427.74	Joback Method
cpg	237.89	J/mol×K	461.79	Joback Method
cpg	251.64	J/mol×K	495.83	Joback Method
cpg	264.82	J/mol×K	529.88	Joback Method
cpg	277.41	J/mol×K	563.93	Joback Method
cpg	289.41	J/mol×K	597.97	Joback Method
cpg	300.83	J/mol×K	632.02	Joback Method

dvisc	0.0038487	Pa×s	235.99	Joback Method
dvisc	0.0021146	Pa×s	267.95	Joback Method
dvisc	0.0013200	Pa×s	299.91	Joback Method
dvisc	0.0009023	Pa×s	331.87	Joback Method
dvisc	0.0006594	Pa×s	363.82	Joback Method
dvisc	0.0005069	Pa×s	395.78	Joback Method
dvisc	0.0004053	Pa×s	427.74	Joback Method

Sources

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=C1499021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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