trans-1,3,5-Cyclohexanetricarboxylic acid, trimethyl ester

Inchi: InChI=1S/C12H18O6/c1-16-10(13)7-4-8(11(14)17-2)6-9(5-7)12(15)18-3/h7-9H,4-6H2,1-3

InchiKey: ZZNOMLSSCRBRJS-FBJIGQNJSA-N

Formula: C12H18O6

SMILES: COC(=O)C1CC(C(=O)OC)CC(C(=O)OC)C1

Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
gf	-642.57	kJ/mol	Joback Method
hf	-1011.77	kJ/mol	Joback Method
hfus	29.17	kJ/mol	Joback Method
hvap	69.58	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.538		Crippen Method
mcvol	191.400	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	713.04	K	Joback Method
tc	922.38	K	Joback Method
tf	440.38	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.12	J/mol×K	713.04	Joback Method
cpg	630.42	J/mol×K	887.49	Joback Method
cpg	618.86	J/mol×K	852.60	Joback Method
cpg	606.12	J/mol×K	817.71	Joback Method
cpg	592.23	J/mol×K	782.82	Joback Method
cpg	577.23	J/mol×K	747.93	Joback Method
cpg	640.78	J/mol×K	922.38	Joback Method
dvisc	0.0001832	Pa×s	713.04	Joback Method
dvisc	0.0002255	Pa×s	667.60	Joback Method

dvisc	0.0002860	Pa×s	622.15	Joback Method
dvisc	0.0003767	Pa×s	576.71	Joback Method
dvisc	0.0005200	Pa×s	531.27	Joback Method
dvisc	0.0007625	Pa×s	485.82	Joback Method
dvisc	0.0012100	Pa×s	440.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R96436&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume