

cis-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-AYMMMOKOSA-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	1791.00		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/molxK	713.04	Joback Method
cpg	577.23	J/molxK	747.93	Joback Method
cpg	592.23	J/molxK	782.82	Joback Method
cpg	606.12	J/molxK	817.71	Joback Method
cpg	618.86	J/molxK	852.60	Joback Method
cpg	630.42	J/molxK	887.49	Joback Method
cpg	640.78	J/molxK	922.38	Joback Method
dvisc	0.0012100	Paxs	440.38	Joback Method
dvisc	0.0007625	Paxs	485.82	Joback Method

dvisc	0.0005200	Paxs	531.27	Joback Method
dvisc	0.0003767	Paxs	576.71	Joback Method
dvisc	0.0002860	Paxs	622.15	Joback Method
dvisc	0.0002255	Paxs	667.60	Joback Method
dvisc	0.0001832	Paxs	713.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R96418&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
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
mccvol:	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

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