1-Propene-1,2,3-tricarboxylic acid, trimethyl ester

Other names:	Trimethyl aconitate
	1,2,3-Propenetricarboxylic acid, trimethyl ester
	3-Methoxycarbonyl-pent-2-enedioic acid dimethyl ester
	Trimethyl 1-propene-1,2,3-tricarboxylate
	Aconitic acid, trimethyl ester
Inchi:	InChI=1S/C9H12O6/c1-13-7(10)4-6(9(12)15-3)5-8(11)14-2/h4H,5H2,1-3H3
InchiKey:	DZAIBGWGBBQGPZ-UHFFFAOYSA-N
Formula:	C9H12O6
SMILES:	COC(=O)C=C(CC(=O)OC)C(=O)OC
Mol. weight [g/mol]:	216.19
CAS:	20820-77-3

Physical Properties

Property code	Value	Unit	Source
gf	-605.19	kJ/mol	Joback Method
hf	-856.06	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-0.03		Crippen Method
logp	-0.178		Crippen Method
mcvol	155.690	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
tb	638.23	K	Joback Method
tc	836.65	K	Joback Method
tf	388.63	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.26	J/mol×K	638.23	Joback Method
cpg	398.25	J/mol×K	671.30	Joback Method

cpg	408.67	J/mol×K	704.37	Joback Method
cpg	418.53	J/mol×K	737.44	Joback Method
cpg	427.81	J/mol×K	770.51	Joback Method
cpg	436.49	J/mol×K	803.58	Joback Method
cpg	444.57	J/mol×K	836.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20820773&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

Legend

cpg:	Ideal gas heat capacity
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

Latest version available from:

https://www.chemeo.com/cid/48-201-5/1-Propene-1-2-3-tricarboxylic-acid-trimethyl-ester.pdf

Generated by Cheméo on 2024-10-12 06:34:34.721153409 +0000 UTC m=+3295737.358122658.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.