

1,1,2-Ethanetricarboxylic acid, triethyl ester

Other names:	Ethane-1,1,2-tricarboxylic acid, triethyl ester Triethyl ethane tricarboxylate Triethyl ethane-1,2,2-tricarboxylate 1,1,2-Tricarbethoxyethane Triethyl 1,1,2-ethanetricarboxylate triethyl ethane-1,1,2-tricarboxylate
Inchi:	InChI=1S/C11H18O6/c1-4-15-9(12)7-8(10(13)16-5-2)11(14)17-6-3/h8H,4-7H2,1-3H3
InchiKey:	TVWZLLYAJDSSCJ-UHFFFAOYSA-N
Formula:	C11H18O6
SMILES:	CCOC(=O)CC(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]:	246.26
CAS:	7459-46-3

Physical Properties

Property code	Value	Unit	Source
gf	-662.46	kJ/mol	Joback Method
hf	-1010.05	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.682		Crippen Method
mcvol	188.170	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	679.51	K	Joback Method
tc	867.80	K	Joback Method
tf	415.21	K	Joback Method
vc	0.718	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.77	J/mol×K	679.51	Joback Method
cpg	568.83	J/mol×K	836.42	Joback Method
cpg	558.62	J/mol×K	805.04	Joback Method

cpg	547.70	J/molxK	773.66	Joback Method
cpg	536.07	J/molxK	742.27	Joback Method
cpg	523.76	J/molxK	710.89	Joback Method
cpg	578.31	J/molxK	867.80	Joback Method
dvisc	0.0001226	Paxs	679.51	Joback Method
dvisc	0.0001580	Paxs	635.46	Joback Method
dvisc	0.0002115	Paxs	591.41	Joback Method
dvisc	0.0002968	Paxs	547.36	Joback Method
dvisc	0.0004418	Paxs	503.31	Joback Method
dvisc	0.0007099	Paxs	459.26	Joback Method
dvisc	0.0012616	Paxs	415.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	0.07	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7459463&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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