1,3,5-Benzenetricarboxylic acid, triethyl ester

Other names: Triethyl trimesate
Triethyl 1,3,5-benzenetricarboxylate
Trimesic acid triethyl ester
Inchi: InChI=1S/C15H18O6/c1-4-19-13(16)10-7-11(14(17)20-5-2)9-12(8-10)15(18)21-6-3/h7-9H
InchiKey: KXGOWZRHSOJOLF-UHFFFAOYSA-N
Formula: C15H18O6
SMILES: CCOC(=O)c1cc(C(=O)OCC)cc(C(=O)OCC)c1
Mol. weight [g/mol]: 294.30
CAS: 4105-92-4

Physical Properties

Property code	Value	Unit	Source
gf	-533.19	kJ/mol	Joback Method
hf	-873.74	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.217		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2066.00		NIST Webbook
rinpol	2066.00		NIST Webbook
tb	808.11	K	Joback Method
tc	1018.00	K	Joback Method
tf	526.75	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.51	J/mol×K	808.11	Joback Method
cpg	647.19	J/mol×K	843.09	Joback Method
cpg	658.83	J/mol×K	878.07	Joback Method
cpg	669.43	J/mol×K	913.05	Joback Method

cpg	678.96	J/mol×K	948.03	Joback Method
cpg	687.42	J/mol×K	983.02	Joback Method
cpg	694.80	J/mol×K	1018.00	Joback Method
dvisc	0.0004943	Pa×s	526.75	Joback Method
dvisc	0.0003221	Pa×s	573.64	Joback Method
dvisc	0.0002240	Pa×s	620.54	Joback Method
dvisc	0.0001639	Pa×s	667.43	Joback Method
dvisc	0.0001250	Pa×s	714.32	Joback Method
dvisc	0.0000985	Pa×s	761.22	Joback Method
dvisc	0.0000798	Pa×s	808.11	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4105924&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
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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