1,3,5-Benzenetricarboxylic acid, triphenyl ester

Other names: Trimesic acid, triphenyl ester
Inchi: InChI=1S/C27H18O6/c28-25(31-22-10-4-1-5-11-22)19-16-20(26(29)32-23-12-6-2-7-13-2
InchiKey: ZNOKZTBEFWQAHD-UHFFFAOYSA-N
Formula: C27H18O6
SMILES: O=C(Oc1ccccc1)c1cc(C(=O)Oc2ccccc2)cc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]: 438.43
CAS: 7383-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-94.92	kJ/mol	Joback Method
hf	-411.83	kJ/mol	Joback Method
hfus	49.43	kJ/mol	Joback Method
hvap	113.59	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	5.344		Crippen Method
mcvol	318.570	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
tb	1162.71	K	Joback Method
tc	1436.10	K	Joback Method
tf	741.25	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.76	J/mol×K	1162.71	Joback Method
cpg	992.58	J/mol×K	1390.53	Joback Method
cpg	994.58	J/mol×K	1344.97	Joback Method
cpg	995.09	J/mol×K	1299.40	Joback Method
cpg	994.03	J/mol×K	1253.84	Joback Method
cpg	991.28	J/mol×K	1208.27	Joback Method
cpg	989.19	J/mol×K	1436.10	Joback Method
dvisc	0.0000157	Pa×s	1162.71	Joback Method

dvisc	0.0000196	Pa×s	1092.47	Joback Method
dvisc	0.0000252	Pa×s	1022.22	Joback Method
dvisc	0.0000336	Pa×s	951.98	Joback Method
dvisc	0.0000469	Pa×s	881.74	Joback Method
dvisc	0.0000694	Pa×s	811.49	Joback Method
dvisc	0.0001106	Pa×s	741.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7383702&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume