1,2,3-Benzenetricarboxylic acid, trimethyl ester

Other names: Benzene-1,2,3-tricarboxylic acid, trimethyl ester
Inchi: InChI=1S/C12H12O6/c1-16-10(13)7-5-4-6-8(11(14)17-2)9(7)12(15)18-3/h4-6H,1-3H3
InchiKey: SBOCVSUCRFVXFE-UHFFFAOYSA-N
Formula: C12H12O6
SMILES: COC(=O)c1cccc(C(=O)OC)c1C(=O)OC
Mol. weight [g/mol]: 252.22
CAS: 2672-57-3

Physical Properties

Property code	Value	Unit	Source
gf	-558.45	kJ/mol	Joback Method
hf	-811.82	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.046		Crippen Method
mcvol	178.500	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	1827.70		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1827.70		NIST Webbook
tb	739.47	K	Joback Method
tc	956.11	K	Joback Method
tf	375.20 ± 0.20	K	NIST Webbook
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.23	J/mol×K	956.11	Joback Method
cpg	473.46	J/mol×K	739.47	Joback Method
cpg	485.01	J/mol×K	775.58	Joback Method
cpg	495.68	J/mol×K	811.68	Joback Method
cpg	505.47	J/mol×K	847.79	Joback Method

cpg	514.34	J/mol×K	883.89	Joback Method
cpg	522.27	J/mol×K	920.00	Joback Method
dvisc	0.0001164	Pa×s	739.47	Joback Method
dvisc	0.0006214	Pa×s	492.94	Joback Method
dvisc	0.0004222	Pa×s	534.03	Joback Method
dvisc	0.0003031	Pa×s	575.12	Joback Method
dvisc	0.0002275	Pa×s	616.21	Joback Method
dvisc	0.0001770	Pa×s	657.29	Joback Method
dvisc	0.0001418	Pa×s	698.38	Joback Method
hfust	32.70	kJ/mol	375.70	NIST Webbook
hvapt	72.50	kJ/mol	483.00	NIST Webbook

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=C2672573&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
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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