Benzenehexacarboxylic acid, hexamethyl ester

Other names: Hexamethyl benzenehexacarboxylate
Hexamethyl mellitate
Mellitic acid, hexamethyl ester

Inchi: InChI=1S/C18H18O12/c1-25-13(19)7-8(14(20)26-2)10(16(22)28-4)12(18(24)30-6)11(17(

InchiKey: BQLICNRRYLYEDI-UHFFFAOYSA-N

Formula: C18H18O12

SMILES: COC(=O)c1c(C(=O)OC)c(C(=O)OC)c(C(=O)OC)c(C(=O)OC)c1C(=O)OC

Mol. weight [g/mol]: 426.33

CAS: 6237-59-8

Physical Properties

Property code	Value	Unit	Source
chs	-7544.80 ± 1.70	kJ/mol	NIST Webbook
gf	-1238.58	kJ/mol	Joback Method
hf	-1704.47	kJ/mol	Joback Method
hfs	-2110.80 ± 1.90	kJ/mol	NIST Webbook
hfus	51.19	kJ/mol	Joback Method
hsub	154.30 ± 1.20	kJ/mol	NIST Webbook
hvap	116.18	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	0.406		Crippen Method
mcvol	285.360	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	1120.56	K	Joback Method
tc	1372.35	K	Joback Method
tf	463.70 ± 0.20	K	NIST Webbook
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.08	J/mol×K	1330.38	Joback Method
cpg	823.47	J/mol×K	1372.35	Joback Method

cpg	873.47	J/mol×K	1120.56	Joback Method
cpg	873.00	J/mol×K	1162.52	Joback Method
cpg	869.55	J/mol×K	1204.49	Joback Method
cpg	863.00	J/mol×K	1246.45	Joback Method
cpg	853.21	J/mol×K	1288.42	Joback Method
dvisc	0.0000196	Pa×s	1120.56	Joback Method
dvisc	0.0000232	Pa×s	1069.57	Joback Method
dvisc	0.0000745	Pa×s	814.60	Joback Method
dvisc	0.0000559	Pa×s	865.59	Joback Method
dvisc	0.0000432	Pa×s	916.59	Joback Method
dvisc	0.0000344	Pa×s	967.58	Joback Method
dvisc	0.0000279	Pa×s	1018.57	Joback Method
hfust	22.50	kJ/mol	463.70	NIST Webbook
hsubt	140.70 ± 1.10	kJ/mol	412.50	NIST Webbook

Sources

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=C6237598&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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