Benzenepentacarboxylic acid, pentamethyl ester

Inchi: InChI=1S/C16H16O10/c1-22-12(17)7-6-8(13(18)23-2)10(15(20)25-4)11(16(21)26-5)9(7)1

InchiKey: UVKUTUMTHIGYKO-UHFFFAOYSA-N

Formula: C16H16O10

SMILES: COC(=O)c1cc(C(=O)OC)c(C(=O)OC)c(C(=O)OC)c1C(=O)OC

Mol. weight [g/mol]: 368.29

CAS: 3327-06-8

Physical Properties

Property code	Value	Unit	Source
chs	-6794.70 ± 1.40	kJ/mol	NIST Webbook
gf	-1011.87	kJ/mol	Joback Method
hf	-1406.92	kJ/mol	Joback Method
hfs	-1788.20 ± 1.60	kJ/mol	NIST Webbook
hfus	43.62	kJ/mol	Joback Method
hsub	165.10 ± 0.80	kJ/mol	NIST Webbook
hsub	165.10 ± 0.80	kJ/mol	NIST Webbook
hvap	101.91	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	0.620		Crippen Method
mcvol	249.740	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	993.53	K	Joback Method
tc	1221.44	K	Joback Method
tf	424.70 ± 0.10	K	NIST Webbook
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.26	J/mol×K	1183.46	Joback Method
cpg	761.06	J/mol×K	1221.44	Joback Method
cpg	750.46	J/mol×K	993.53	Joback Method

cpg	756.96	J/mol×K	1031.52	Joback Method
cpg	761.66	J/mol×K	1069.50	Joback Method
cpg	764.49	J/mol×K	1107.49	Joback Method
cpg	765.38	J/mol×K	1145.47	Joback Method
dvisc	0.0000371	Pa×s	993.53	Joback Method
dvisc	0.0000443	Pa×s	945.84	Joback Method
dvisc	0.0001536	Pa×s	707.38	Joback Method
dvisc	0.0001125	Pa×s	755.07	Joback Method
dvisc	0.0000855	Pa×s	802.76	Joback Method
dvisc	0.0000670	Pa×s	850.45	Joback Method
dvisc	0.0000539	Pa×s	898.15	Joback Method
hfust	38.00	kJ/mol	424.70	NIST Webbook
hsubt	160.00 ± 0.80	kJ/mol	401.00	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=C3327068&Units=SI

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

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