1,2,4,5-Benzene-tetracarboxylic acid tetrapropyl EsTEr

Inchi: InChI=1S/C22H30O8/c1-5-9-27-19(23)15-13-17(21(25)29-11-7-3)18(22(26)30-12-8-4)14
InchiKey: SAMCWPHEYXOOMA-UHFFFAOYSA-N
Formula: C22H30O8
SMILES: CCCOC(=O)c1cc(C(=O)OCCC)c(C(=O)OCCC)cc1C(=O)OCCC
Mol. weight [g/mol]: 422.47
CAS: 3143-08-6

Physical Properties

Property code	Value	Unit	Source
chl	-11295.60 ± 3.50	kJ/mol	NIST Webbook
gf	-717.80	kJ/mol	Joback Method
hf	-1581.50	kJ/mol	NIST Webbook
hf	-1546.00 ± 7.00	kJ/mol	NIST Webbook
hfl	-1649.10 ± 3.70	kJ/mol	NIST Webbook
hfl	-1613.60 ± 3.50	kJ/mol	NIST Webbook
hfus	56.76	kJ/mol	Joback Method
hvap	67.60	kJ/mol	NIST Webbook
log10ws	-5.79		Crippen Method
logp	3.954		Crippen Method
mcvol	326.840	ml/mol	McGowan Method
pc	1222.55	kPa	Joback Method
tb	1049.54	K	Joback Method
tc	1285.44	K	Joback Method
tf	690.32	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.07	J/mol×K	1049.54	Joback Method
cpg	1081.94	J/mol×K	1088.86	Joback Method
cpg	1089.77	J/mol×K	1128.17	Joback Method
cpg	1095.53	J/mol×K	1167.49	Joback Method
cpg	1099.22	J/mol×K	1206.80	Joback Method

cpg	1100.80	J/mol×K	1246.12	Joback Method
cpg	1100.26	J/mol×K	1285.44	Joback Method
dvisc	0.0001345	Pa×s	690.32	Joback Method
dvisc	0.0000874	Pa×s	750.19	Joback Method
dvisc	0.0000605	Pa×s	810.06	Joback Method
dvisc	0.0000440	Pa×s	869.93	Joback Method
dvisc	0.0000334	Pa×s	929.80	Joback Method
dvisc	0.0000262	Pa×s	989.67	Joback Method
dvisc	0.0000211	Pa×s	1049.54	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=C3143086&Units=SI

Legend

chl: Standard liquid 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
hfl: Liquid phase 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

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