

1,2,4,5-Benzene-tetracarboxylic acid, dipropyl ester

Inchi:	InChI=1S/C16H18O8/c1-3-5-23-15(21)11-7-10(14(19)20)12(8-9(11)13(17)18)16(22)24-6
InchiKey:	UMPAINQRYDYVBA-UHFFFAOYSA-N
Formula:	C16H18O8
SMILES:	CCCOC(=O)c1cc(C(=O)O)c(C(=O)OCCC)cc1C(=O)O
Mol. weight [g/mol]:	338.31
CAS:	56941-72-1

Physical Properties

Property code	Value	Unit	Source
chs	-7224.40 ± 2.30	kJ/mol	NIST Webbook
gf	-831.96	kJ/mol	Joback Method
hf	-1190.67	kJ/mol	Joback Method
hfs	-1644.20 ± 2.60	kJ/mol	NIST Webbook
hfus	47.02	kJ/mol	Joback Method
hvap	120.63	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.217		Crippen Method
mcvol	242.300	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
tb	1051.78	K	Joback Method
tc	1288.97	K	Joback Method
tf	699.88	K	Joback Method
vc	0.921	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.12	J/mol×K	1051.78	Joback Method
cpg	764.63	J/mol×K	1091.31	Joback Method
cpg	769.81	J/mol×K	1130.84	Joback Method
cpg	773.65	J/mol×K	1170.38	Joback Method
cpg	776.16	J/mol×K	1209.91	Joback Method
cpg	777.33	J/mol×K	1249.44	Joback Method
cpg	777.18	J/mol×K	1288.97	Joback Method

dvisc	0.0000259	Paxs	699.88	Joback Method
dvisc	0.0000128	Paxs	758.53	Joback Method
dvisc	0.0000070	Paxs	817.18	Joback Method
dvisc	0.0000042	Paxs	875.83	Joback Method
dvisc	0.0000026	Paxs	934.48	Joback Method
dvisc	0.0000018	Paxs	993.13	Joback Method
dvisc	0.0000012	Paxs	1051.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56941721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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