Diethyl pyromellitate

Inchi: InChI=1S/C14H14O8/c1-3-21-13(19)9-5-8(12(17)18)10(14(20)22-4-2)6-7(9)11(15)16/h5-
InchiKey: FKBDSZNRJFOVHK-UHFFFAOYSA-N
Formula: C14H14O8
SMILES: CCOC(=O)c1cc(C(=O)O)c(C(=O)OCC)cc1C(=O)O
Mol. weight [g/mol]: 310.26
CAS: 50853-29-7

Physical Properties

Property code	Value	Unit	Source
chs	-5917.40 ± 1.90	kJ/mol	NIST Webbook
gf	-848.80	kJ/mol	Joback Method
hf	-1149.39	kJ/mol	Joback Method
hfs	-1592.60 ± 1.90	kJ/mol	NIST Webbook
hfus	41.84	kJ/mol	Joback Method
hvap	116.18	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	1.436		Crippen Method
mcvol	214.120	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
tb	1006.02	K	Joback Method
tc	1231.78	K	Joback Method
tf	677.34	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.46	J/mol×K	1006.02	Joback Method
cpg	651.59	J/mol×K	1043.65	Joback Method
cpg	656.60	J/mol×K	1081.27	Joback Method
cpg	660.49	J/mol×K	1118.90	Joback Method
cpg	663.25	J/mol×K	1156.52	Joback Method
cpg	664.87	J/mol×K	1194.15	Joback Method
cpg	665.35	J/mol×K	1231.78	Joback Method

dvisc	0.0000363	Pa×s	677.34	Joback Method
dvisc	0.0000183	Pa×s	732.12	Joback Method
dvisc	0.0000102	Pa×s	786.90	Joback Method
dvisc	0.0000061	Pa×s	841.68	Joback Method
dvisc	0.0000039	Pa×s	896.46	Joback Method
dvisc	0.0000026	Pa×s	951.24	Joback Method
dvisc	0.0000018	Pa×s	1006.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50853297&Units=SI
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

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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