Adipic acid, ethyl 2,3,5,6-tetrachlorophenyl ester

Inchi: InChI=1S/C14H14Cl4O4/c1-2-21-10(19)5-3-4-6-11(20)22-14-12(17)8(15)7-9(16)13(14)18

InchiKey: BDBBXGBXIOCULM-UHFFFAOYSA-N

Formula: C14H14Cl4O4

SMILES: CCOC(=O)CCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl

Mol. weight [g/mol]: 388.07

Physical Properties

Property code	Value	Unit	Source
gf	-374.67	kJ/mol	Joback Method
hf	-694.20	kJ/mol	Joback Method
hfus	46.86	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.329		Crippen Method
mcvol	248.200	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2491.00		NIST Webbook
tb	868.62	K	Joback Method
tc	1090.59	K	Joback Method
tf	588.04	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.71	J/mol×K	868.62	Joback Method
cpg	638.47	J/mol×K	905.61	Joback Method
cpg	647.28	J/mol×K	942.61	Joback Method
cpg	655.12	J/mol×K	979.60	Joback Method
cpg	662.00	J/mol×K	1016.60	Joback Method
cpg	667.90	J/mol×K	1053.59	Joback Method
cpg	672.83	J/mol×K	1090.59	Joback Method
dvisc	0.0003601	Pa×s	588.04	Joback Method
dvisc	0.0002511	Pa×s	634.80	Joback Method

dvisc	0.0001839	Pa×s	681.57	Joback Method
dvisc	0.0001403	Pa×s	728.33	Joback Method
dvisc	0.0001105	Pa×s	775.09	Joback Method
dvisc	0.0000894	Pa×s	821.86	Joback Method
dvisc	0.0000741	Pa×s	868.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353945&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume