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

Inchi: InChI=1S/C16H18Cl4O4/c1-9(2)8-23-12(21)5-3-4-6-13(22)24-16-14(19)10(17)7-11(18)15

InchiKey: IBKJTWOUNXFHHO-UHFFFAOYSA-N

Formula: C16H18Cl4O4

SMILES: CC(C)COC(=O)CCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl

Mol. weight [g/mol]: 416.12

Physical Properties

Property code	Value	Unit	Source
gf	-360.27	kJ/mol	Joback Method
hf	-740.76	kJ/mol	Joback Method
hfus	48.52	kJ/mol	Joback Method
hvap	91.60	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.965		Crippen Method
mcvol	276.380	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2644.00		NIST Webbook
tb	913.94	K	Joback Method
tc	1136.40	K	Joback Method
tf	595.58	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.33	J/mol×K	913.94	Joback Method
cpg	781.34	J/mol×K	1099.33	Joback Method
cpg	775.31	J/mol×K	1062.25	Joback Method
cpg	768.20	J/mol×K	1025.17	Joback Method
cpg	760.00	J/mol×K	988.09	Joback Method
cpg	750.72	J/mol×K	951.02	Joback Method
cpg	786.29	J/mol×K	1136.40	Joback Method
dvisc	0.0000507	Pa×s	913.94	Joback Method
dvisc	0.0000625	Pa×s	860.88	Joback Method

dvisc	0.0000792	Pa×s	807.82	Joback Method
dvisc	0.0001038	Pa×s	754.76	Joback Method
dvisc	0.0001417	Pa×s	701.70	Joback Method
dvisc	0.0002035	Pa×s	648.64	Joback Method
dvisc	0.0003117	Pa×s	595.58	Joback Method

Sources

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=U353947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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