Adipic acid, isohexyl 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C18H22Cl4O4/c1-11(2)6-5-9-25-14(23)7-3-4-8-15(24)26-18-13(20)10-12(19)16

InchiKey: WNZIYHGVWGWMLF-UHFFFAOYSA-N

Formula: C18H22Cl4O4

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

Mol. weight [g/mol]: 444.18

Physical Properties

Property code	Value	Unit	Source
gf	-343.43	kJ/mol	Joback Method
hf	-782.04	kJ/mol	Joback Method
hfus	53.70	kJ/mol	Joback Method
hvap	96.05	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.745		Crippen Method
mcvol	304.560	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
tb	959.70	K	Joback Method
tc	1182.94	K	Joback Method
tf	618.12	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.34	J/mol×K	959.70	Joback Method
cpg	865.10	J/mol×K	996.91	Joback Method
cpg	874.65	J/mol×K	1034.11	Joback Method
cpg	883.01	J/mol×K	1071.32	Joback Method
cpg	890.19	J/mol×K	1108.52	Joback Method
cpg	896.21	J/mol×K	1145.73	Joback Method
cpg	901.06	J/mol×K	1182.94	Joback Method
dvisc	0.0002506	Pa×s	618.12	Joback Method

dvisc	0.0001599	Pa×s	675.05	Joback Method
dvisc	0.0001094	Pa×s	731.98	Joback Method
dvisc	0.0000791	Pa×s	788.91	Joback Method
dvisc	0.0000597	Pa×s	845.84	Joback Method
dvisc	0.0000467	Pa×s	902.77	Joback Method
dvisc	0.0000376	Pa×s	959.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353916&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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