Adipic acid, di(2,3,6-trichlorophenyl) ester

Inchi: InChI=1S/C18H12Cl6O4/c19-9-5-7-11(21)17(15(9)23)27-13(25)3-1-2-4-14(26)28-18-12(
InchiKey: DGDGCCSZGSQLHP-UHFFFAOYSA-N
Formula: C18H12Cl6O4
SMILES: O=C(CCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 505.00

Physical Properties

Property code	Value	Unit	Source
gf	-271.70	kJ/mol	Joback Method
hf	-594.65	kJ/mol	Joback Method
hfus	58.88	kJ/mol	Joback Method
hvap	108.81	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.678		Crippen Method
mcvol	305.280	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	3514.00		NIST Webbook
tb	1071.64	K	Joback Method
tc	1324.29	K	Joback Method
tf	744.42	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.19	J/mol×K	1071.64	Joback Method
cpg	774.35	J/mol×K	1113.75	Joback Method
cpg	778.17	J/mol×K	1155.86	Joback Method
cpg	780.67	J/mol×K	1197.96	Joback Method
cpg	781.87	J/mol×K	1240.07	Joback Method
cpg	781.78	J/mol×K	1282.18	Joback Method
cpg	780.42	J/mol×K	1324.29	Joback Method
dvisc	0.0001363	Pa×s	744.42	Joback Method
dvisc	0.0000986	Pa×s	798.96	Joback Method

dvisc	0.0000744	Pa×s	853.49	Joback Method
dvisc	0.0000580	Pa×s	908.03	Joback Method
dvisc	0.0000465	Pa×s	962.57	Joback Method
dvisc	0.0000382	Pa×s	1017.10	Joback Method
dvisc	0.0000320	Pa×s	1071.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353944&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