Adipic acid, propyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C15H17Cl3O4/c1-2-9-21-12(19)5-3-4-6-13(20)22-15-11(17)8-7-10(16)14(15)18
InchiKey: WESRAKJUWWHBNZ-UHFFFAOYSA-N
Formula: C15H17Cl3O4
SMILES: CCCOC(=O)CCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 367.65

Physical Properties

Property code	Value	Unit	Source
gf	-344.69	kJ/mol	Joback Method
hf	-687.63	kJ/mol	Joback Method
hfus	45.64	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.066		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2440.00		NIST Webbook
tb	849.09	K	Joback Method
tc	1065.19	K	Joback Method
tf	556.87	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.65	J/mol×K	849.09	Joback Method
cpg	675.93	J/mol×K	885.11	Joback Method
cpg	686.23	J/mol×K	921.12	Joback Method
cpg	695.56	J/mol×K	957.14	Joback Method
cpg	703.92	J/mol×K	993.16	Joback Method
cpg	711.31	J/mol×K	1029.18	Joback Method
cpg	717.74	J/mol×K	1065.19	Joback Method
dvisc	0.0004288	Pa×s	556.87	Joback Method
dvisc	0.0002840	Pa×s	605.57	Joback Method

dvisc	0.0002000	Pa×s	654.28	Joback Method
dvisc	0.0001478	Pa×s	702.98	Joback Method
dvisc	0.0001137	Pa×s	751.68	Joback Method
dvisc	0.0000902	Pa×s	800.39	Joback Method
dvisc	0.0000735	Pa×s	849.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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