Adipic acid, pentyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C17H21Cl3O4/c1-2-3-6-9-23-15(21)7-4-5-8-16(22)24-14-11-12(18)10-13(19)17
InchiKey: YQYWLJCJWMTIHR-UHFFFAOYSA-N
Formula: C17H21Cl3O4
SMILES: CCCCCOC(=O)CCCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 395.70

Physical Properties

Property code	Value	Unit	Source
gf	-327.85	kJ/mol	Joback Method
hf	-728.91	kJ/mol	Joback Method
hfus	50.82	kJ/mol	Joback Method
hvap	89.16	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.846		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2633.00		NIST Webbook
tb	894.85	K	Joback Method
tc	1109.82	K	Joback Method
tf	579.41	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.95	J/mol×K	894.85	Joback Method
cpg	788.76	J/mol×K	930.68	Joback Method
cpg	799.50	J/mol×K	966.51	Joback Method
cpg	809.18	J/mol×K	1002.34	Joback Method
cpg	817.80	J/mol×K	1038.17	Joback Method
cpg	825.39	J/mol×K	1073.99	Joback Method
cpg	831.96	J/mol×K	1109.82	Joback Method
dvisc	0.0003515	Pa×s	579.41	Joback Method
dvisc	0.0002271	Pa×s	631.98	Joback Method

dvisc	0.0001570	Pa×s	684.56	Joback Method
dvisc	0.0001143	Pa×s	737.13	Joback Method
dvisc	0.0000869	Pa×s	789.70	Joback Method
dvisc	0.0000683	Pa×s	842.28	Joback Method
dvisc	0.0000553	Pa×s	894.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353869&Units=SI

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