Dodecanoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C18H24Cl4O2/c1-2-3-4-5-6-7-8-9-10-11-15(23)24-18-14(20)12-13(19)16(21)17

InchiKey: AKCVHXIPDUOGKY-UHFFFAOYSA-N

Formula: C18H24Cl4O2

SMILES: CCCCCCCCCCCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 414.19

Physical Properties

Property code	Value	Unit	Source
gf	-107.07	kJ/mol	Joback Method
hf	-531.96	kJ/mol	Joback Method
hfus	54.44	kJ/mol	Joback Method
hvap	87.28	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.127		Crippen Method
mcvol	297.120	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	2589.00		NIST Webbook
tb	883.85	K	Joback Method
tc	1096.29	K	Joback Method
tf	560.96	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.46	J/mol×K	883.85	Joback Method
cpg	874.53	J/mol×K	1060.88	Joback Method
cpg	865.17	J/mol×K	1025.48	Joback Method
cpg	854.91	J/mol×K	990.07	Joback Method
cpg	843.72	J/mol×K	954.66	Joback Method
cpg	831.58	J/mol×K	919.26	Joback Method
cpg	883.01	J/mol×K	1096.29	Joback Method
dvisc	0.0000582	Pa×s	883.85	Joback Method
dvisc	0.0000719	Pa×s	830.03	Joback Method

dvisc	0.0000915	Pa×s	776.22	Joback Method
dvisc	0.0001207	Pa×s	722.40	Joback Method
dvisc	0.0001665	Pa×s	668.59	Joback Method
dvisc	0.0002431	Pa×s	614.77	Joback Method
dvisc	0.0003814	Pa×s	560.96	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=U360550&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