Lauric acid, pentachlorophenyl ester

Other names: pentachlorophenyl laurate
Inchi: InChI=1S/C18H23Cl5O2/c1-2-3-4-5-6-7-8-9-10-11-12(24)25-18-16(22)14(20)13(19)15(21
InchiKey: MKNJWAXSYGAMGJ-UHFFFAOYSA-N
Formula: C18H23Cl5O2
SMILES: CCCCCCCCCCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 448.64
CAS: 3772-94-9

Physical Properties

Property code	Value	Unit	Source
gf	-128.63	kJ/mol	Joback Method
hf	-559.17	kJ/mol	Joback Method
hfus	58.24	kJ/mol	Joback Method
hvap	92.33	kJ/mol	Joback Method
log10ws	-9.40		Crippen Method
logp	8.780		Crippen Method
mcvol	309.360	ml/mol	McGowan Method
pc	1249.49	kPa	Joback Method
tb	926.26	K	Joback Method
tc	1144.44	K	Joback Method
tf	603.40	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.81	J/mol×K	926.26	Joback Method
cpg	890.07	J/mol×K	1108.07	Joback Method
cpg	881.92	J/mol×K	1071.71	Joback Method
cpg	872.84	J/mol×K	1035.35	Joback Method
cpg	862.82	J/mol×K	998.99	Joback Method
cpg	851.82	J/mol×K	962.62	Joback Method
cpg	897.33	J/mol×K	1144.44	Joback Method
dvisc	0.0000506	Pa×s	926.26	Joback Method

dvisc	0.0000618	Pa×s	872.45	Joback Method
dvisc	0.0000775	Pa×s	818.64	Joback Method
dvisc	0.0001004	Pa×s	764.83	Joback Method
dvisc	0.0001351	Pa×s	711.02	Joback Method
dvisc	0.0001911	Pa×s	657.21	Joback Method
dvisc	0.0002873	Pa×s	603.40	Joback Method

Sources

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=C3772949&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume