

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

Inchi:	InChI=1S/C15H18Cl4O2/c1-2-3-4-5-6-7-8-12(20)21-15-11(17)9-10(16)13(18)14(15)19/h
InchiKey:	BGFFVJAUWJUQAE-UHFFFAOYSA-N
Formula:	C15H18Cl4O2
SMILES:	CCCCCCCCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	372.11

Physical Properties

Property code	Value	Unit	Source
gf	-132.33	kJ/mol	Joback Method
hf	-470.04	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.956		Crippen Method
mcvol	254.850	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinsol	2411.00		NIST Webbook
tb	815.21	K	Joback Method
tc	1030.17	K	Joback Method
tf	527.15	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.62	J/molxK	815.21	Joback Method
cpg	661.77	J/molxK	851.04	Joback Method
cpg	673.04	J/molxK	886.86	Joback Method
cpg	683.46	J/molxK	922.69	Joback Method
cpg	693.04	J/molxK	958.52	Joback Method
cpg	701.80	J/molxK	994.34	Joback Method
cpg	709.76	J/molxK	1030.17	Joback Method
dvisc	0.0005067	Paxs	527.15	Joback Method
dvisc	0.0003355	Paxs	575.16	Joback Method

dvisc	0.0002367	Paxs	623.17	Joback Method
dvisc	0.0001755	Paxs	671.18	Joback Method
dvisc	0.0001354	Paxs	719.19	Joback Method
dvisc	0.0001080	Paxs	767.20	Joback Method
dvisc	0.0000884	Paxs	815.21	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=U360674&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

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