

Adipic acid, pentyl 2,3,5,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C17H20Cl4O4/c1-2-3-6-9-24-13(22)7-4-5-8-14(23)25-17-15(20)11(18)10-12(19)
InchiKey:	SXXJTXQWXMMGLE-UHFFFAOYSA-N
Formula:	C17H20Cl4O4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	430.15

Physical Properties

Property code	Value	Unit	Source
gf	-349.41	kJ/mol	Joback Method
hf	-756.12	kJ/mol	Joback Method
hfus	54.63	kJ/mol	Joback Method
hvap	94.21	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.499		Crippen Method
mvol	290.470	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2778.00		NIST Webbook
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tb	937.26	K	Joback Method
tc	1157.93	K	Joback Method
tf	621.85	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.49	J/molxK	937.26	Joback Method
cpg	807.04	J/molxK	974.04	Joback Method
cpg	816.47	J/molxK	1010.82	Joback Method
cpg	824.79	J/molxK	1047.59	Joback Method
cpg	832.01	J/molxK	1084.37	Joback Method
cpg	838.14	J/molxK	1121.15	Joback Method
cpg	843.19	J/molxK	1157.93	Joback Method
dvisc	0.0002652	Paxs	621.85	Joback Method

dvisc	0.0001784	Paxs	674.42	Joback Method
dvisc	0.0001271	Paxs	726.99	Joback Method
dvisc	0.0000948	Paxs	779.56	Joback Method
dvisc	0.0000734	Paxs	832.12	Joback Method
dvisc	0.0000586	Paxs	884.69	Joback Method
dvisc	0.0000479	Paxs	937.26	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=U353949&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
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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