

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

Inchi:	InChI=1S/C19H24Cl4O4/c1-2-3-4-5-8-11-26-15(24)9-6-7-10-16(25)27-19-17(22)13(20)12
InchiKey:	FHWUNBJZTLWJAU-UHFFFAOYSA-N
Formula:	C19H24Cl4O4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	458.20

Physical Properties

Property code	Value	Unit	Source
gf	-332.57	kJ/mol	Joback Method
hf	-797.40	kJ/mol	Joback Method
hfus	59.81	kJ/mol	Joback Method
hvap	98.66	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.280		Crippen Method
mvol	318.650	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2997.00		NIST Webbook
rinpol	2997.00		NIST Webbook
tb	983.02	K	Joback Method
tc	1206.91	K	Joback Method
tf	644.39	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.87	J/molxK	983.02	Joback Method
cpg	922.78	J/molxK	1020.34	Joback Method
cpg	932.46	J/molxK	1057.65	Joback Method
cpg	940.91	J/molxK	1094.97	Joback Method
cpg	948.16	J/molxK	1132.28	Joback Method
cpg	954.21	J/molxK	1169.60	Joback Method
cpg	959.09	J/molxK	1206.91	Joback Method
dvisc	0.0002127	Paxs	644.39	Joback Method

dvisc	0.0001400	Paxs	700.83	Joback Method
dvisc	0.0000980	Paxs	757.27	Joback Method
dvisc	0.0000721	Paxs	813.71	Joback Method
dvisc	0.0000552	Paxs	870.14	Joback Method
dvisc	0.0000437	Paxs	926.58	Joback Method
dvisc	0.0000355	Paxs	983.02	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=U353952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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