

Sebacic acid, hexyl 2,3,5,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C22H30Cl4O4/c1-2-3-4-11-14-29-18(27)12-9-7-5-6-8-10-13-19(28)30-22-20(2)
InchiKey:	IRIJTHQPBYIEGU-UHFFFAOYSA-N
Formula:	C22H30Cl4O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	500.28

Physical Properties

Property code	Value	Unit	Source
gf	-307.31	kJ/mol	Joback Method
hf	-859.32	kJ/mol	Joback Method
hfus	67.58	kJ/mol	Joback Method
hvap	105.34	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.450		Crippen Method
mcvol	360.920	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	3357.00		NIST Webbook
rinpol	3357.00		NIST Webbook
tb	1051.66	K	Joback Method
tc	1287.64	K	Joback Method
tf	678.20	K	Joback Method
vc	1.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.01	J/molxK	1051.66	Joback Method
cpg	1100.39	J/molxK	1090.99	Joback Method
cpg	1110.27	J/molxK	1130.32	Joback Method
cpg	1118.70	J/molxK	1169.65	Joback Method
cpg	1125.71	J/molxK	1208.98	Joback Method
cpg	1131.32	J/molxK	1248.31	Joback Method
cpg	1135.56	J/molxK	1287.64	Joback Method
dvisc	0.0001497	Paxs	678.20	Joback Method

dvisc	0.0000954	Paxs	740.44	Joback Method
dvisc	0.0000652	Paxs	802.69	Joback Method
dvisc	0.0000471	Paxs	864.93	Joback Method
dvisc	0.0000355	Paxs	927.17	Joback Method
dvisc	0.0000278	Paxs	989.42	Joback Method
dvisc	0.0000223	Paxs	1051.66	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=U355294&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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