

Sebacic acid, heptyl 2,3,4,5-tetrachlorophenyl ester

Inchi:	InChI=1S/C23H32Cl4O4/c1-2-3-4-9-12-15-30-19(28)13-10-7-5-6-8-11-14-20(29)31-18-16
InchiKey:	RYGUCRGFYQQVQL-UHFFFAOYSA-N
Formula:	C23H32Cl4O4
SMILES:	CCCCCCCC(=O)CCCCCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	514.31

Physical Properties

Property code	Value	Unit	Source
gf	-298.89	kJ/mol	Joback Method
hf	-879.96	kJ/mol	Joback Method
hfus	70.17	kJ/mol	Joback Method
hvap	107.57	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.840		Crippen Method
mcvol	375.010	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	3539.00		NIST Webbook
rinpol	3539.00		NIST Webbook
tb	1074.54	K	Joback Method
tc	1316.76	K	Joback Method
tf	689.47	K	Joback Method
vc	1.460	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.94	J/molxK	1074.54	Joback Method
cpg	1190.95	J/molxK	1276.39	Joback Method
cpg	1185.59	J/molxK	1236.02	Joback Method
cpg	1178.74	J/molxK	1195.65	Joback Method
cpg	1170.37	J/molxK	1155.28	Joback Method
cpg	1160.45	J/molxK	1114.91	Joback Method
cpg	1194.88	J/molxK	1316.76	Joback Method
dvisc	0.0000191	Paxs	1074.54	Joback Method

dvisc	0.0000238	Paxs	1010.36	Joback Method
dvisc	0.0000306	Paxs	946.18	Joback Method
dvisc	0.0000407	Paxs	882.00	Joback Method
dvisc	0.0000567	Paxs	817.83	Joback Method
dvisc	0.0000836	Paxs	753.65	Joback Method
dvisc	0.0001324	Paxs	689.47	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=U355287&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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