Sebacic acid, isohexyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C22H31Cl3O4/c1-16(2)10-9-13-28-20(26)11-7-5-3-4-6-8-12-21(27)29-22-18(24

InchiKey: YHAHBHNWPFZMFJ-UHFFFAOYSA-N

Formula: C22H31Cl3O4

SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 465.84

Physical Properties

Property code	Value	Unit	Source
gf	-288.19	kJ/mol	Joback Method
hf	-837.39	kJ/mol	Joback Method
hfus	60.25	kJ/mol	Joback Method
hvap	99.91	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.652		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	3118.00		NIST Webbook
tb	1008.81	K	Joback Method
tc	1235.42	K	Joback Method
tf	620.76	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.25	J/mol×K	1008.81	Joback Method
cpg	1082.97	J/mol×K	1046.58	Joback Method
cpg	1094.29	J/mol×K	1084.35	Joback Method
cpg	1104.24	J/mol×K	1122.12	Joback Method
cpg	1112.84	J/mol×K	1159.88	Joback Method
cpg	1120.13	J/mol×K	1197.65	Joback Method
cpg	1126.15	J/mol×K	1235.42	Joback Method
dvisc	0.0002140	Pa×s	620.76	Joback Method
dvisc	0.0001248	Pa×s	685.43	Joback Method

dvisc	0.0000798	Pa×s	750.11	Joback Method
dvisc	0.0000548	Pa×s	814.78	Joback Method
dvisc	0.0000398	Pa×s	879.46	Joback Method
dvisc	0.0000302	Pa×s	944.13	Joback Method
dvisc	0.0000237	Pa×s	1008.81	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=U355079&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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