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

Inchi: InChI=1S/C20H26Cl4O4/c1-13(2)12-27-16(25)9-7-5-3-4-6-8-10-17(26)28-20-18(23)14(21
InchiKey: VTZNJJZJUFHXDE-UHFFFAOYSA-N
Formula: C20H26Cl4O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 472.23

Physical Properties

Property code	Value	Unit	Source
gf	-326.59	kJ/mol	Joback Method
hf	-823.32	kJ/mol	Joback Method
hfus	58.88	kJ/mol	Joback Method
hvap	100.50	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.526		Crippen Method
mcvol	332.740	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	3111.00		NIST Webbook
rinpol	3111.00		NIST Webbook
tb	1005.46	K	Joback Method
tc	1232.98	K	Joback Method
tf	640.66	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.82	J/mol×K	1005.46	Joback Method
cpg	981.86	J/mol×K	1043.38	Joback Method
cpg	991.56	J/mol×K	1081.30	Joback Method
cpg	999.95	J/mol×K	1119.22	Joback Method
cpg	1007.05	J/mol×K	1157.14	Joback Method
cpg	1012.88	J/mol×K	1195.06	Joback Method
cpg	1017.45	J/mol×K	1232.98	Joback Method
dvisc	0.0001990	Pa×s	640.66	Joback Method

dvisc	0.0001243	Pa×s	701.46	Joback Method
dvisc	0.0000836	Pa×s	762.26	Joback Method
dvisc	0.0000597	Pa×s	823.06	Joback Method
dvisc	0.0000446	Pa×s	883.86	Joback Method
dvisc	0.0000346	Pa×s	944.66	Joback Method
dvisc	0.0000277	Pa×s	1005.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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