Sebacic acid, isobutyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C20H27Cl3O4/c1-14(2)13-26-19(24)9-7-5-3-4-6-8-10-20(25)27-18-12-16(22)15
InchiKey: IQTIBDLIYVIXQQ-UHFFFAOYSA-N
Formula: C20H27Cl3O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 437.79

Physical Properties

Property code	Value	Unit	Source
gf	-305.03	kJ/mol	Joback Method
hf	-796.11	kJ/mol	Joback Method
hfus	55.07	kJ/mol	Joback Method
hvap	95.45	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.872		Crippen Method
mcvol	320.500	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2944.00		NIST Webbook
tb	963.05	K	Joback Method
tc	1183.13	K	Joback Method
tf	598.22	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.38	J/mol×K	963.05	Joback Method
cpg	1001.06	J/mol×K	1146.45	Joback Method
cpg	993.57	J/mol×K	1109.77	Joback Method
cpg	984.87	J/mol×K	1073.09	Joback Method
cpg	974.96	J/mol×K	1036.41	Joback Method
cpg	963.80	J/mol×K	999.73	Joback Method
cpg	1007.39	J/mol×K	1183.13	Joback Method
dvisc	0.0000323	Pa×s	963.05	Joback Method
dvisc	0.0000408	Pa×s	902.24	Joback Method

dvisc	0.0000534	Pa×s	841.44	Joback Method
dvisc	0.0000729	Pa×s	780.63	Joback Method
dvisc	0.0001049	Pa×s	719.83	Joback Method
dvisc	0.0001614	Pa×s	659.02	Joback Method
dvisc	0.0002711	Pa×s	598.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355192&Units=SI

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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