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

Inchi: InChI=1S/C20H27Cl3O4/c1-14(2)13-26-18(24)9-7-5-3-4-6-8-10-19(25)27-20-16(22)11-15

InchiKey: UPKPXWIKPFSLLE-UHFFFAOYSA-N

Formula: C20H27Cl3O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1c(Cl)cc(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	2889.00		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	963.80	J/mol×K	999.73	Joback Method
cpg	974.96	J/mol×K	1036.41	Joback Method
cpg	984.87	J/mol×K	1073.09	Joback Method
cpg	993.57	J/mol×K	1109.77	Joback Method
cpg	1001.06	J/mol×K	1146.45	Joback Method
cpg	1007.39	J/mol×K	1183.13	Joback Method
dvisc	0.0002711	Pa×s	598.22	Joback Method
dvisc	0.0001614	Pa×s	659.02	Joback Method

dvisc	0.0001049	Pa×s	719.83	Joback Method
dvisc	0.0000729	Pa×s	780.63	Joback Method
dvisc	0.0000534	Pa×s	841.44	Joback Method
dvisc	0.0000408	Pa×s	902.24	Joback Method
dvisc	0.0000323	Pa×s	963.05	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=U355076&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