Sebacic acid, propyl 2,4,6-trichlorobenzyl ester

Inchi: InChI=1S/C20H27Cl3O4/c1-2-11-26-19(24)9-7-5-3-4-6-8-10-20(25)27-14-16-17(22)12-15

InchiKey: ZSRHIIVBSGTQHF-UHFFFAOYSA-N

Formula: C20H27Cl3O4

SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 437.79

Physical Properties

Property code	Value	Unit	Source
gf	-302.59	kJ/mol	Joback Method
hf	-790.83	kJ/mol	Joback Method
hfus	58.59	kJ/mol	Joback Method
hvap	95.84	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.764		Crippen Method
mcvol	320.500	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
tb	963.49	K	Joback Method
tc	1182.62	K	Joback Method
tf	613.22	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.93	J/mol×K	963.49	Joback Method
cpg	963.35	J/mol×K	1000.01	Joback Method
cpg	974.53	J/mol×K	1036.53	Joback Method
cpg	984.50	J/mol×K	1073.05	Joback Method
cpg	993.26	J/mol×K	1109.58	Joback Method
cpg	1000.85	J/mol×K	1146.10	Joback Method
cpg	1007.29	J/mol×K	1182.62	Joback Method
dvisc	0.0002540	Pa×s	613.22	Joback Method

dvisc	0.0001586	Pa×s	671.60	Joback Method
dvisc	0.0001068	Pa×s	729.98	Joback Method
dvisc	0.0000762	Pa×s	788.36	Joback Method
dvisc	0.0000570	Pa×s	846.73	Joback Method
dvisc	0.0000442	Pa×s	905.11	Joback Method
dvisc	0.0000354	Pa×s	963.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380572&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

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