

Sebacic acid, isobutyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C20H27Cl3O4/c1-14(2)13-26-18(24)9-7-5-3-4-6-8-10-19(25)27-15-11-16(21)20
InchiKey:	IVJYZLXXDZTOEX-UHFFFAOYSA-N
Formula:	C20H27Cl3O4
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
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
rinpola	3013.00		NIST Webbook
tb	963.05	K	Joback Method
tc	1183.13	K	Joback Method
tf	598.22	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.38	J/molxK	963.05	Joback Method
cpg	963.80	J/molxK	999.73	Joback Method
cpg	974.96	J/molxK	1036.41	Joback Method
cpg	984.87	J/molxK	1073.09	Joback Method
cpg	993.57	J/molxK	1109.77	Joback Method
cpg	1001.06	J/molxK	1146.45	Joback Method
cpg	1007.39	J/molxK	1183.13	Joback Method
dvisc	0.0002711	Paxs	598.22	Joback Method
dvisc	0.0001614	Paxs	659.02	Joback Method

dvisc	0.0001049	Paxs	719.83	Joback Method
dvisc	0.0000729	Paxs	780.63	Joback Method
dvisc	0.0000534	Paxs	841.44	Joback Method
dvisc	0.0000408	Paxs	902.24	Joback Method
dvisc	0.0000323	Paxs	963.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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