

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

Inchi:	InChI=1S/C20H26Cl4O4/c1-2-3-12-27-16(25)10-8-6-4-5-7-9-11-17(26)28-20-18(23)14(2)
InchiKey:	OPMBYUPWSYXJCV-UHFFFAOYSA-N
Formula:	C20H26Cl4O4
SMILES:	CCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	472.23

Physical Properties

Property code	Value	Unit	Source
gf	-324.15	kJ/mol	Joback Method
hf	-818.04	kJ/mol	Joback Method
hfus	62.40	kJ/mol	Joback Method
hvap	100.89	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.670		Crippen Method
mcvol	332.740	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	3158.00		NIST Webbook
tb	1005.90	K	Joback Method
tc	1232.79	K	Joback Method
tf	655.66	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.43	J/molxK	1005.90	Joback Method
cpg	981.50	J/molxK	1043.72	Joback Method
cpg	991.27	J/molxK	1081.53	Joback Method
cpg	999.74	J/molxK	1119.35	Joback Method
cpg	1006.95	J/molxK	1157.16	Joback Method
cpg	1012.90	J/molxK	1194.98	Joback Method
cpg	1017.62	J/molxK	1232.79	Joback Method
dvisc	0.0001897	Paxs	655.66	Joback Method
dvisc	0.0001235	Paxs	714.03	Joback Method

dvisc	0.0000858	Paxs	772.41	Joback Method
dvisc	0.0000627	Paxs	830.78	Joback Method
dvisc	0.0000478	Paxs	889.15	Joback Method
dvisc	0.0000376	Paxs	947.53	Joback Method
dvisc	0.0000305	Paxs	1005.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355291&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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