

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

Inchi:	InChI=1S/C14H14Cl4O4/c1-2-3-6-21-10(19)4-5-11(20)22-14-12(17)8(15)7-9(16)13(14)18
InchiKey:	SONGAIHAYOVDSW-UHFFFAOYSA-N
Formula:	C14H14Cl4O4
SMILES:	CCCCOC(=O)CCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	388.07

Physical Properties

Property code	Value	Unit	Source
gf	-374.67	kJ/mol	Joback Method
hf	-694.20	kJ/mol	Joback Method
hfus	46.86	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.329		Crippen Method
mvol	248.200	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2473.00		NIST Webbook
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tb	868.62	K	Joback Method
tc	1090.59	K	Joback Method
tf	588.04	K	Joback Method
vc	0.956	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.71	J/molxK	868.62	Joback Method
cpg	638.47	J/molxK	905.61	Joback Method
cpg	647.28	J/molxK	942.61	Joback Method
cpg	655.12	J/molxK	979.60	Joback Method
cpg	662.00	J/molxK	1016.60	Joback Method
cpg	667.90	J/molxK	1053.59	Joback Method
cpg	672.83	J/molxK	1090.59	Joback Method
dvisc	0.0003601	Paxs	588.04	Joback Method

dvisc	0.0002511	Paxs	634.80	Joback Method
dvisc	0.0001839	Paxs	681.57	Joback Method
dvisc	0.0001403	Paxs	728.33	Joback Method
dvisc	0.0001105	Paxs	775.09	Joback Method
dvisc	0.0000894	Paxs	821.86	Joback Method
dvisc	0.0000741	Paxs	868.62	Joback Method

Sources

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=U353317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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