Succinic acid, octyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C18H23Cl3O4/c1-2-3-4-5-6-7-12-24-15(22)10-11-16(23)25-18-14(20)9-8-13(19
InchiKey: XEYNTLMQFHCOLE-UHFFFAOYSA-N
Formula: C18H23Cl3O4
SMILES: CCCCCCCCOC(=O)CCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 409.73

Physical Properties

Property code	Value	Unit	Source
gf	-319.43	kJ/mol	Joback Method
hf	-749.55	kJ/mol	Joback Method
hfus	53.41	kJ/mol	Joback Method
hvap	91.39	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.236		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	917.73	K	Joback Method
tc	1133.26	K	Joback Method
tf	590.68	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.27	J/mol×K	917.73	Joback Method
cpg	846.30	J/mol×K	953.65	Joback Method
cpg	857.21	J/mol×K	989.57	Joback Method
cpg	867.01	J/mol×K	1025.49	Joback Method
cpg	875.72	J/mol×K	1061.41	Joback Method
cpg	883.34	J/mol×K	1097.33	Joback Method
cpg	889.90	J/mol×K	1133.26	Joback Method
dvisc	0.0003165	Pa×s	590.68	Joback Method

dvisc	0.0002021	Pa×s	645.19	Joback Method
dvisc	0.0001384	Pa×s	699.70	Joback Method
dvisc	0.0001001	Pa×s	754.21	Joback Method
dvisc	0.0000757	Pa×s	808.71	Joback Method
dvisc	0.0000592	Pa×s	863.22	Joback Method
dvisc	0.0000477	Pa×s	917.73	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=U349709&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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