Succinic acid, 2,3-dichlorophenyl 2-octyl ester

Inchi: InChI=1S/C18H24Cl2O4/c1-3-4-5-6-8-13(2)23-16(21)11-12-17(22)24-15-10-7-9-14(19)18
InchiKey: MBUBVOBAFMVCTP-UHFFFAOYSA-N
Formula: C18H24Cl2O4
SMILES: CCCCCCC(C)OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 375.29

Physical Properties

Property code	Value	Unit	Source
gf	-300.31	kJ/mol	Joback Method
hf	-727.62	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	85.96	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.581		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2462.00		NIST Webbook
tb	874.88	K	Joback Method
tc	1086.47	K	Joback Method
tf	533.24	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.01	J/mol×K	874.88	Joback Method
cpg	868.92	J/mol×K	1051.21	Joback Method
cpg	859.90	J/mol×K	1015.94	Joback Method
cpg	849.82	J/mol×K	980.68	Joback Method
cpg	838.66	J/mol×K	945.41	Joback Method
cpg	826.39	J/mol×K	910.15	Joback Method
cpg	876.88	J/mol×K	1086.47	Joback Method
dvisc	0.0000503	Pa×s	874.88	Joback Method
dvisc	0.0000641	Pa×s	817.94	Joback Method

dvisc	0.0000847	Pa×s	761.00	Joback Method
dvisc	0.0001172	Pa×s	704.06	Joback Method
dvisc	0.0001716	Pa×s	647.12	Joback Method
dvisc	0.0002706	Pa×s	590.18	Joback Method
dvisc	0.0004701	Pa×s	533.24	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=U370981&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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