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

Inchi: InChI=1S/C15H18Cl2O4/c1-3-10(4-2)20-13(18)8-9-14(19)21-12-7-5-6-11(16)15(12)17/h5

InchiKey: NJHJXQQJVVRSRI-UHFFFAOYSA-N

Formula: C15H18Cl2O4

SMILES: CCC(CC)OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 333.21

Physical Properties

Property code	Value	Unit	Source
gf	-325.57	kJ/mol	Joback Method
hf	-665.70	kJ/mol	Joback Method
hfus	38.31	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.411		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2184.00		NIST Webbook
tb	806.24	K	Joback Method
tc	1020.76	K	Joback Method
tf	499.43	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.00	J/mol×K	806.24	Joback Method
cpg	656.65	J/mol×K	841.99	Joback Method
cpg	668.30	J/mol×K	877.75	Joback Method
cpg	678.96	J/mol×K	913.50	Joback Method
cpg	688.64	J/mol×K	949.25	Joback Method
cpg	697.34	J/mol×K	985.00	Joback Method
cpg	705.08	J/mol×K	1020.76	Joback Method
dvisc	0.0006347	Pa×s	499.43	Joback Method
dvisc	0.0003791	Pa×s	550.57	Joback Method

dvisc	0.0002472	Pa×s	601.70	Joback Method
dvisc	0.0001723	Pa×s	652.84	Joback Method
dvisc	0.0001266	Pa×s	703.97	Joback Method
dvisc	0.0000970	Pa×s	755.11	Joback Method
dvisc	0.0000769	Pa×s	806.24	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=U370921&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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