Succinic acid, 2,4,6-trichlorophenyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H17Cl3O5/c24-16-12-19(25)23(20(26)13-16)31-22(28)10-9-21(27)29-14-1

InchiKey: LLZYSLJTYXECJV-UHFFFAOYSA-N

Formula: C23H17Cl3O5

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 479.74

Physical Properties

Property code	Value	Unit	Source
gf	-167.14	kJ/mol	Joback Method
hf	-523.38	kJ/mol	Joback Method
hfus	55.25	kJ/mol	Joback Method
hvap	110.14	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	6.868		Crippen Method
mcvol	321.120	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook
tb	1112.89	K	Joback Method
tc	1372.61	K	Joback Method
tf	734.62	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.99	J/mol×K	1112.89	Joback Method
cpg	929.63	J/mol×K	1329.32	Joback Method
cpg	930.73	J/mol×K	1286.04	Joback Method
cpg	930.26	J/mol×K	1242.75	Joback Method
cpg	928.17	J/mol×K	1199.46	Joback Method
cpg	924.43	J/mol×K	1156.18	Joback Method
cpg	926.99	J/mol×K	1372.61	Joback Method
dvisc	0.0000185	Pa×s	1112.89	Joback Method

dvisc	0.0000226	Pa×s	1049.84	Joback Method
dvisc	0.0000284	Pa×s	986.80	Joback Method
dvisc	0.0000368	Pa×s	923.75	Joback Method
dvisc	0.0000495	Pa×s	860.71	Joback Method
dvisc	0.0000698	Pa×s	797.67	Joback Method
dvisc	0.0001044	Pa×s	734.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390380&Units=SI
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

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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