Succinic acid, 3-chlorophenyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H19ClO5/c24-18-7-5-11-21(15-18)29-23(26)13-12-22(25)27-16-17-6-4-10-

InchiKey: DSCGAGNYRDXVON-UHFFFAOYSA-N

Formula: C23H19ClO5

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 410.85

Physical Properties

Property code	Value	Unit	Source
gf	-124.02	kJ/mol	Joback Method
hf	-468.96	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	100.05	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.561		Crippen Method
mcvol	296.640	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	3174.00		NIST Webbook
rinpol	3174.00		NIST Webbook
tb	1028.07	K	Joback Method
tc	1277.85	K	Joback Method
tf	649.74	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.20	J/mol×K	1028.07	Joback Method
cpg	902.39	J/mol×K	1069.70	Joback Method
cpg	909.96	J/mol×K	1111.33	Joback Method
cpg	915.96	J/mol×K	1152.96	Joback Method
cpg	920.46	J/mol×K	1194.59	Joback Method
cpg	923.49	J/mol×K	1236.22	Joback Method
cpg	925.10	J/mol×K	1277.85	Joback Method
dvisc	0.0001794	Pa×s	649.74	Joback Method

dvisc	0.0001113	Pa×s	712.79	Joback Method
dvisc	0.0000747	Pa×s	775.85	Joback Method
dvisc	0.0000532	Pa×s	838.90	Joback Method
dvisc	0.0000397	Pa×s	901.96	Joback Method
dvisc	0.0000308	Pa×s	965.01	Joback Method
dvisc	0.0000247	Pa×s	1028.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390375&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