Succinic acid, 2,2-dichloroethyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C19H18Cl2O5/c20-17(21)13-25-19(23)10-9-18(22)24-12-14-5-4-8-16(11-14)26

InchiKey: SCCKPNHCCSKRRT-UHFFFAOYSA-N

Formula: C19H18Cl2O5

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

Mol. weight [g/mol]: 397.25

Physical Properties

Property code	Value	Unit	Source
gf	-274.85	kJ/mol	Joback Method
hf	-632.48	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	92.21	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.649		Crippen Method
mcvol	276.280	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	2816.00		NIST Webbook
rinpol	2816.00		NIST Webbook
tb	941.88	K	Joback Method
tc	1176.13	K	Joback Method
tf	580.64	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.83	J/mol×K	941.88	Joback Method
cpg	834.15	J/mol×K	1137.09	Joback Method
cpg	828.96	J/mol×K	1098.05	Joback Method
cpg	822.45	J/mol×K	1059.01	Joback Method
cpg	814.62	J/mol×K	1019.96	Joback Method
cpg	805.42	J/mol×K	980.92	Joback Method
cpg	838.07	J/mol×K	1176.13	Joback Method
dvisc	0.0000325	Pa×s	941.88	Joback Method

dvisc	0.0000415	Pa×s	881.67	Joback Method
dvisc	0.0000548	Pa×s	821.47	Joback Method
dvisc	0.0000757	Pa×s	761.26	Joback Method
dvisc	0.0001106	Pa×s	701.05	Joback Method
dvisc	0.0001733	Pa×s	640.85	Joback Method
dvisc	0.0002982	Pa×s	580.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390368&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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