Succinic acid, 2,4-dichlorobenzyl hexyl ester

Inchi: InChI=1S/C17H22Cl2O4/c1-2-3-4-5-10-22-16(20)8-9-17(21)23-12-13-6-7-14(18)11-15(13
InchiKey: XHHMHWDFXKDAAK-UHFFFAOYSA-N
Formula: C17H22Cl2O4
SMILES: CCCCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 361.26

Physical Properties

Property code	Value	Unit	Source
gf	-306.29	kJ/mol	Joback Method
hf	-701.70	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.940		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2477.00		NIST Webbook
tb	852.44	K	Joback Method
tc	1062.07	K	Joback Method
tf	536.97	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.26	J/mol×K	852.44	Joback Method
cpg	768.31	J/mol×K	887.38	Joback Method
cpg	780.32	J/mol×K	922.32	Joback Method
cpg	791.29	J/mol×K	957.25	Joback Method
cpg	801.26	J/mol×K	992.19	Joback Method
cpg	810.22	J/mol×K	1027.13	Joback Method
cpg	818.20	J/mol×K	1062.07	Joback Method
dvisc	0.0004746	Pa×s	536.97	Joback Method

dvisc	0.0002921	Pa×s	589.55	Joback Method
dvisc	0.0001947	Pa×s	642.13	Joback Method
dvisc	0.0001380	Pa×s	694.70	Joback Method
dvisc	0.0001026	Pa×s	747.28	Joback Method
dvisc	0.0000794	Pa×s	799.86	Joback Method
dvisc	0.0000634	Pa×s	852.44	Joback Method

Sources

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=U381142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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