Succinic acid, 2,4-dichlorophenethyl hexadecyl ester

Inchi: InChI=1S/C28H44Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-33-27(31)18-19-28(32

InchiKey: YMNCDDPSQZSXGO-UHFFFAOYSA-N

Formula: C28H44Cl2O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 515.55

Physical Properties

Property code	Value	Unit	Source
gf	-213.67	kJ/mol	Joback Method
hf	-928.74	kJ/mol	Joback Method
hfus	75.51	kJ/mol	Joback Method
hvap	108.60	kJ/mol	Joback Method
log10ws	-9.74		Crippen Method
logp	8.884		Crippen Method
mcvol	420.980	ml/mol	McGowan Method
pc	777.21	kPa	Joback Method
rinpol	3580.00		NIST Webbook
rinpol	3580.00		NIST Webbook
tb	1104.12	K	Joback Method
tc	1364.93	K	Joback Method
tf	660.94	K	Joback Method
vc	1.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1417.02	J/mol×K	1104.12	Joback Method
cpg	1432.66	J/mol×K	1147.59	Joback Method
cpg	1446.30	J/mol×K	1191.06	Joback Method
cpg	1458.03	J/mol×K	1234.52	Joback Method
cpg	1467.93	J/mol×K	1277.99	Joback Method
cpg	1476.11	J/mol×K	1321.46	Joback Method
cpg	1482.65	J/mol×K	1364.93	Joback Method
dvisc	0.0001311	Pa×s	660.94	Joback Method

dvisc	0.0000718	Pa×s	734.80	Joback Method
dvisc	0.0000439	Pa×s	808.67	Joback Method
dvisc	0.0000292	Pa×s	882.53	Joback Method
dvisc	0.0000206	Pa×s	956.39	Joback Method
dvisc	0.0000153	Pa×s	1030.26	Joback Method
dvisc	0.0000119	Pa×s	1104.12	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=U381600&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