Sebacic acid, 2-(2-chlorophenoxy)ethyl isobutyl ester

Inchi: InChI=1S/C22H33ClO5/c1-18(2)17-28-22(25)14-8-6-4-3-5-7-13-21(24)27-16-15-26-20-12

InchiKey: ONYCQUXOFUKVRV-UHFFFAOYSA-N

Formula: C22H33ClO5

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCCOc1ccccc1Cl

Mol. weight [g/mol]: 412.95

Physical Properties

Property code	Value	Unit	Source
gf	-350.07	kJ/mol	Joback Method
hf	-915.19	kJ/mol	Joback Method
hfus	53.82	kJ/mol	Joback Method
hvap	92.22	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.582		Crippen Method
mcvol	330.070	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	946.41	K	Joback Method
tc	1160.10	K	Joback Method
tf	558.11	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.48	J/mol×K	946.41	Joback Method
cpg	1068.22	J/mol×K	982.02	Joback Method
cpg	1081.53	J/mol×K	1017.64	Joback Method
cpg	1093.43	J/mol×K	1053.25	Joback Method
cpg	1103.94	J/mol×K	1088.87	Joback Method
cpg	1113.09	J/mol×K	1124.48	Joback Method
cpg	1120.90	J/mol×K	1160.10	Joback Method
dvisc	0.0002959	Pa×s	558.11	Joback Method

dvisc	0.0001562	Pa×s	622.83	Joback Method
dvisc	0.0000930	Pa×s	687.54	Joback Method
dvisc	0.0000605	Pa×s	752.26	Joback Method
dvisc	0.0000422	Pa×s	816.98	Joback Method
dvisc	0.0000310	Pa×s	881.69	Joback Method
dvisc	0.0000237	Pa×s	946.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416772&Units=SI

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