Sebacic acid, 3-chlorophenyl isohexyl ester

Inchi: InChI=1S/C22H33ClO4/c1-18(2)11-10-16-26-21(24)14-7-5-3-4-6-8-15-22(25)27-20-13-9-
InchiKey: VKFODDISUKQPNT-UHFFFAOYSA-N
Formula: C22H33ClO4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-245.07	kJ/mol	Joback Method
hf	-782.97	kJ/mol	Joback Method
hfus	52.64	kJ/mol	Joback Method
hvap	89.81	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.346		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2912.00		NIST Webbook
rinpol	2912.00		NIST Webbook
tb	923.99	K	Joback Method
tc	1134.49	K	Joback Method
tf	535.88	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.82	J/mol×K	923.99	Joback Method
cpg	1089.43	J/mol×K	1099.41	Joback Method
cpg	1078.94	J/mol×K	1064.32	Joback Method
cpg	1067.27	J/mol×K	1029.24	Joback Method
cpg	1054.38	J/mol×K	994.16	Joback Method
cpg	1040.24	J/mol×K	959.07	Joback Method
cpg	1098.78	J/mol×K	1134.49	Joback Method
dvisc	0.0000321	Pa×s	923.99	Joback Method

dvisc	0.0000421	Pa×s	859.30	Joback Method
dvisc	0.0000575	Pa×s	794.62	Joback Method
dvisc	0.0000832	Pa×s	729.93	Joback Method
dvisc	0.0001294	Pa×s	665.25	Joback Method
dvisc	0.0002211	Pa×s	600.57	Joback Method
dvisc	0.0004300	Pa×s	535.88	Joback Method

Sources

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=U354861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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