Sebacic acid, 4-chlorophenethyl pentyl ester

Inchi: InChI=1S/C23H35ClO4/c1-2-3-10-18-27-22(25)11-8-6-4-5-7-9-12-23(26)28-19-17-20-13-
InchiKey: XDHNOMXTAYYQTB-UHFFFAOYSA-N
Formula: C23H35ClO4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCCc1ccc(Cl)cc1
Mol. weight [g/mol]: 410.98

Physical Properties

Property code	Value	Unit	Source
gf	-234.21	kJ/mol	Joback Method
hf	-798.33	kJ/mol	Joback Method
hfus	58.75	kJ/mol	Joback Method
hvap	92.43	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	6.280		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	2956.00		NIST Webbook
rinpol	2956.00		NIST Webbook
tb	947.31	K	Joback Method
tc	1160.48	K	Joback Method
tf	562.15	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.97	J/mol×K	947.31	Joback Method
cpg	1100.59	J/mol×K	982.84	Joback Method
cpg	1114.89	J/mol×K	1018.37	Joback Method
cpg	1127.90	J/mol×K	1053.89	Joback Method
cpg	1139.65	J/mol×K	1089.42	Joback Method
cpg	1150.19	J/mol×K	1124.95	Joback Method
cpg	1159.55	J/mol×K	1160.48	Joback Method
dvisc	0.0003455	Pa×s	562.15	Joback Method

dvisc	0.0001870	Pa×s	626.34	Joback Method
dvisc	0.0001135	Pa×s	690.54	Joback Method
dvisc	0.0000750	Pa×s	754.73	Joback Method
dvisc	0.0000529	Pa×s	818.92	Joback Method
dvisc	0.0000392	Pa×s	883.12	Joback Method
dvisc	0.0000303	Pa×s	947.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416252&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