Sebacic acid, 4-chloro-2-methylphenyl isohexyl ester

Inchi: InChI=1S/C23H35ClO4/c1-18(2)11-10-16-27-22(25)12-8-6-4-5-7-9-13-23(26)28-21-15-14

InchiKey: XZLOYXHSJRVVMK-UHFFFAOYSA-N

Formula: C23H35ClO4

SMILES: Cc1cc(Cl)ccc1OC(=O)CCCCCCCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 410.98

Physical Properties

Property code	Value	Unit	Source
gf	-246.28	kJ/mol	Joback Method
hf	-815.08	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	92.70	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.654		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2953.00		NIST Webbook
tb	951.85	K	Joback Method
tc	1166.48	K	Joback Method
tf	559.67	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.61	J/mol×K	951.85	Joback Method
cpg	1100.12	J/mol×K	987.62	Joback Method
cpg	1114.25	J/mol×K	1023.39	Joback Method
cpg	1127.04	J/mol×K	1059.16	Joback Method
cpg	1138.53	J/mol×K	1094.93	Joback Method
cpg	1148.74	J/mol×K	1130.70	Joback Method
cpg	1157.71	J/mol×K	1166.48	Joback Method
dvisc	0.0003328	Pa×s	559.67	Joback Method
dvisc	0.0001779	Pa×s	625.03	Joback Method

dvisc	0.0001070	Pa×s	690.40	Joback Method
dvisc	0.0000703	Pa×s	755.76	Joback Method
dvisc	0.0000494	Pa×s	821.12	Joback Method
dvisc	0.0000366	Pa×s	886.49	Joback Method
dvisc	0.0000282	Pa×s	951.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355103&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