Sebacic acid, di(2-chloro-5-methylphenyl) ester

Inchi: InChI=1S/C24H28Cl2O4/c1-17-11-13-19(25)21(15-17)29-23(27)9-7-5-3-4-6-8-10-24(28)3

InchiKey: FQMFAHUSZCKPEF-UHFFFAOYSA-N

Formula: C24H28Cl2O4

SMILES: Cc1ccc(Cl)c(OC(=O)CCCCCCCCC(=O)Oc2cc(C)ccc2Cl)c1

Mol. weight [g/mol]: 451.38

Physical Properties

Property code	Value	Unit	Source
gf	-154.20	kJ/mol	Joback Method
hf	-632.59	kJ/mol	Joback Method
hfus	58.41	kJ/mol	Joback Method
hvap	103.30	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	7.242		Crippen Method
mcvol	340.860	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinpol	3455.00		NIST Webbook
tb	1049.24	K	Joback Method
tc	1286.78	K	Joback Method
tf	667.32	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.03	J/mol×K	1049.24	Joback Method
cpg	1097.71	J/mol×K	1247.19	Joback Method
cpg	1092.20	J/mol×K	1207.60	Joback Method
cpg	1085.32	J/mol×K	1168.01	Joback Method
cpg	1077.02	J/mol×K	1128.42	Joback Method
cpg	1067.27	J/mol×K	1088.83	Joback Method
cpg	1101.90	J/mol×K	1286.78	Joback Method
dvisc	0.0000246	Pa×s	1049.24	Joback Method
dvisc	0.0000305	Pa×s	985.59	Joback Method

dvisc	0.0000390	Pa×s	921.93	Joback Method
dvisc	0.0000518	Pa×s	858.28	Joback Method
dvisc	0.0000719	Pa×s	794.63	Joback Method
dvisc	0.0001056	Pa×s	730.97	Joback Method
dvisc	0.0001669	Pa×s	667.32	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=U355310&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