Sebacic acid, 4-chloro-3-methylphenyl octyl ester

Inchi: InChI=1S/C25H39ClO4/c1-3-4-5-6-11-14-19-29-24(27)15-12-9-7-8-10-13-16-25(28)30-22

InchiKey: CUWCTAORMIVXLB-UHFFFAOYSA-N

Formula: C25H39ClO4

SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 439.03

Physical Properties

Property code	Value	Unit	Source
gf	-227.00	kJ/mol	Joback Method
hf	-851.08	kJ/mol	Joback Method
hfus	63.54	kJ/mol	Joback Method
hvap	97.54	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.578		Crippen Method
mcvol	366.470	ml/mol	McGowan Method
pc	939.79	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	998.05	K	Joback Method
tc	1222.32	K	Joback Method
tf	597.21	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.93	J/mol×K	998.05	Joback Method
cpg	1222.93	J/mol×K	1035.43	Joback Method
cpg	1237.39	J/mol×K	1072.81	Joback Method
cpg	1250.36	J/mol×K	1110.18	Joback Method
cpg	1261.89	J/mol×K	1147.56	Joback Method
cpg	1272.01	J/mol×K	1184.94	Joback Method
cpg	1280.79	J/mol×K	1222.32	Joback Method
dvisc	0.0002411	Pa×s	597.21	Joback Method

dvisc	0.0001336	Pa×s	664.02	Joback Method
dvisc	0.0000825	Pa×s	730.82	Joback Method
dvisc	0.0000552	Pa×s	797.63	Joback Method
dvisc	0.0000393	Pa×s	864.44	Joback Method
dvisc	0.0000294	Pa×s	931.24	Joback Method
dvisc	0.0000229	Pa×s	998.05	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=U354850&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