Sebacic acid, 2-chloro-5-methylphenyl undecyl ester

Inchi: InChI=1S/C28H45ClO4/c1-3-4-5-6-7-8-11-14-17-22-32-27(30)18-15-12-9-10-13-16-19-28

InchiKey: WHUNWXUZRKNZSP-UHFFFAOYSA-N

Formula: C28H45ClO4

SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 481.11

Physical Properties

Property code	Value	Unit	Source
gf	-201.74	kJ/mol	Joback Method
hf	-913.00	kJ/mol	Joback Method
hfus	71.31	kJ/mol	Joback Method
hvap	104.22	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.749		Crippen Method
mcvol	408.740	ml/mol	McGowan Method
pc	793.49	kPa	Joback Method
rinpol	3516.00		NIST Webbook
rinpol	3516.00		NIST Webbook
tb	1066.69	K	Joback Method
tc	1314.62	K	Joback Method
tf	631.02	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.04	J/mol×K	1066.69	Joback Method
cpg	1410.91	J/mol×K	1108.01	Joback Method
cpg	1425.85	J/mol×K	1149.33	Joback Method
cpg	1438.95	J/mol×K	1190.66	Joback Method
cpg	1450.28	J/mol×K	1231.98	Joback Method
cpg	1459.92	J/mol×K	1273.30	Joback Method
cpg	1467.94	J/mol×K	1314.62	Joback Method
dvisc	0.0001662	Pa×s	631.02	Joback Method

dvisc	0.0000895	Pa×s	703.63	Joback Method
dvisc	0.0000541	Pa×s	776.24	Joback Method
dvisc	0.0000356	Pa×s	848.86	Joback Method
dvisc	0.0000251	Pa×s	921.47	Joback Method
dvisc	0.0000186	Pa×s	994.08	Joback Method
dvisc	0.0000143	Pa×s	1066.69	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=U355309&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