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

Inchi: InChI=1S/C26H41ClO4/c1-3-4-5-6-9-12-15-20-30-25(28)16-13-10-7-8-11-14-17-26(29)31

InchiKey: YIBNDTHQSOWIHE-UHFFFAOYSA-N

Formula: C26H41ClO4

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

Mol. weight [g/mol]: 453.05

Physical Properties

Property code	Value	Unit	Source
gf	-218.58	kJ/mol	Joback Method
hf	-871.72	kJ/mol	Joback Method
hfus	66.13	kJ/mol	Joback Method
hvap	99.77	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.968		Crippen Method
mcvol	380.560	ml/mol	McGowan Method
pc	886.83	kPa	Joback Method
rinpol	3290.00		NIST Webbook
rinpol	3290.00		NIST Webbook
tb	1020.93	K	Joback Method
tc	1251.86	K	Joback Method
tf	608.48	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.95	J/mol×K	1020.93	Joback Method
cpg	1285.21	J/mol×K	1059.42	Joback Method
cpg	1299.83	J/mol×K	1097.91	Joback Method
cpg	1312.85	J/mol×K	1136.39	Joback Method
cpg	1324.34	J/mol×K	1174.88	Joback Method
cpg	1334.34	J/mol×K	1213.37	Joback Method
cpg	1342.90	J/mol×K	1251.86	Joback Method
dvisc	0.0002135	Pa×s	608.48	Joback Method

dvisc	0.0001172	Pa×s	677.22	Joback Method
dvisc	0.0000718	Pa×s	745.96	Joback Method
dvisc	0.0000478	Pa×s	814.71	Joback Method
dvisc	0.0000339	Pa×s	883.45	Joback Method
dvisc	0.0000253	Pa×s	952.19	Joback Method
dvisc	0.0000196	Pa×s	1020.93	Joback Method

Sources

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=U355307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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