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

Inchi: InChI=1S/C27H43ClO4/c1-3-4-5-6-7-10-13-16-21-31-26(29)17-14-11-8-9-12-15-18-27(30

InchiKey: MNLHUUSGIFCMIH-UHFFFAOYSA-N

Formula: C27H43ClO4

SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 467.08

Physical Properties

Property code	Value	Unit	Source
gf	-210.16	kJ/mol	Joback Method
hf	-892.36	kJ/mol	Joback Method
hfus	68.72	kJ/mol	Joback Method
hvap	101.99	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.359		Crippen Method
mcvol	394.650	ml/mol	McGowan Method
pc	838.21	kPa	Joback Method
rinpol	3406.00		NIST Webbook
rinpol	3406.00		NIST Webbook
tb	1043.81	K	Joback Method
tc	1282.60	K	Joback Method
tf	619.75	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.33	J/mol×K	1043.81	Joback Method
cpg	1347.88	J/mol×K	1083.61	Joback Method
cpg	1362.66	J/mol×K	1123.41	Joback Method
cpg	1375.73	J/mol×K	1163.20	Joback Method
cpg	1387.15	J/mol×K	1203.00	Joback Method
cpg	1396.99	J/mol×K	1242.80	Joback Method
cpg	1405.30	J/mol×K	1282.60	Joback Method
dvisc	0.0001886	Pa×s	619.75	Joback Method

dvisc	0.0001025	Pa×s	690.43	Joback Method
dvisc	0.0000624	Pa×s	761.10	Joback Method
dvisc	0.0000413	Pa×s	831.78	Joback Method
dvisc	0.0000292	Pa×s	902.46	Joback Method
dvisc	0.0000217	Pa×s	973.13	Joback Method
dvisc	0.0000168	Pa×s	1043.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355108&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