Sebacic acid, 2-(2-chlorophenoxy)ethyl decyl ester

Inchi: InChI=1S/C28H45ClO5/c1-2-3-4-5-6-9-12-17-22-33-27(30)20-13-10-7-8-11-14-21-28(31)

InchiKey: VLTDRPHWDMDXMZ-UHFFFAOYSA-N

Formula: C28H45ClO5

SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1Cl

Mol. weight [g/mol]: 497.11

Physical Properties

Property code	Value	Unit	Source
gf	-297.11	kJ/mol	Joback Method
hf	-1033.75	kJ/mol	Joback Method
hfus	72.89	kJ/mol	Joback Method
hvap	105.97	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.067		Crippen Method
mcvol	414.610	ml/mol	McGowan Method
pc	792.60	kPa	Joback Method
rinpol	3322.00		NIST Webbook
rinpol	3322.00		NIST Webbook
tb	1084.13	K	Joback Method
tc	1340.28	K	Joback Method
tf	640.73	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.13	J/mol×K	1084.13	Joback Method
cpg	1479.89	J/mol×K	1297.59	Joback Method
cpg	1472.50	J/mol×K	1254.89	Joback Method
cpg	1463.10	J/mol×K	1212.20	Joback Method
cpg	1451.62	J/mol×K	1169.51	Joback Method
cpg	1437.99	J/mol×K	1126.82	Joback Method
cpg	1485.33	J/mol×K	1340.28	Joback Method
dvisc	0.0000102	Pa×s	1084.13	Joback Method

dvisc	0.0000133	Pa×s	1010.23	Joback Method
dvisc	0.0000181	Pa×s	936.33	Joback Method
dvisc	0.0000260	Pa×s	862.43	Joback Method
dvisc	0.0000399	Pa×s	788.53	Joback Method
dvisc	0.0000671	Pa×s	714.63	Joback Method
dvisc	0.0001271	Pa×s	640.73	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=U416779&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