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

Inchi: InChI=1S/C25H39ClO5/c1-2-3-4-9-14-19-30-24(27)17-10-7-5-6-8-11-18-25(28)31-21-20-

InchiKey: FIIPCUNMVSPJKP-UHFFFAOYSA-N

Formula: C25H39ClO5

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

Mol. weight [g/mol]: 455.03

Physical Properties

Property code	Value	Unit	Source
gf	-322.37	kJ/mol	Joback Method
hf	-971.83	kJ/mol	Joback Method
hfus	65.12	kJ/mol	Joback Method
hvap	99.29	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.896		Crippen Method
mcvol	372.340	ml/mol	McGowan Method
pc	938.64	kPa	Joback Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
tb	1015.49	K	Joback Method
tc	1244.83	K	Joback Method
tf	606.92	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1236.03	J/mol×K	1015.49	Joback Method
cpg	1251.30	J/mol×K	1053.71	Joback Method
cpg	1264.84	J/mol×K	1091.94	Joback Method
cpg	1276.68	J/mol×K	1130.16	Joback Method
cpg	1286.87	J/mol×K	1168.39	Joback Method
cpg	1295.45	J/mol×K	1206.61	Joback Method
cpg	1302.45	J/mol×K	1244.83	Joback Method
dvisc	0.0001873	Pa×s	606.92	Joback Method

dvisc	0.0001016	Pa×s	675.02	Joback Method
dvisc	0.0000617	Pa×s	743.11	Joback Method
dvisc	0.0000407	Pa×s	811.20	Joback Method
dvisc	0.0000287	Pa×s	879.30	Joback Method
dvisc	0.0000212	Pa×s	947.39	Joback Method
dvisc	0.0000164	Pa×s	1015.49	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=U416776&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