Sebacic acid, decyl 2,5-dichlorobenzyl ester

Inchi: InChI=1S/C27H42Cl2O4/c1-2-3-4-5-6-9-12-15-20-32-26(30)16-13-10-7-8-11-14-17-27(31
InchiKey: UMLBKMKXGAPJNY-UHFFFAOYSA-N
Formula: C27H42Cl2O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 501.53

Physical Properties

Property code	Value	Unit	Source
gf	-222.09	kJ/mol	Joback Method
hf	-908.10	kJ/mol	Joback Method
hfus	72.92	kJ/mol	Joback Method
hvap	106.38	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	8.841		Crippen Method
mcvol	406.890	ml/mol	McGowan Method
pc	820.54	kPa	Joback Method
rinpol	3498.00		NIST Webbook
rinpol	3498.00		NIST Webbook
tb	1081.24	K	Joback Method
tc	1331.71	K	Joback Method
tf	649.67	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.70	J/mol×K	1081.24	Joback Method
cpg	1370.04	J/mol×K	1122.98	Joback Method
cpg	1383.53	J/mol×K	1164.73	Joback Method
cpg	1395.25	J/mol×K	1206.47	Joback Method
cpg	1405.28	J/mol×K	1248.22	Joback Method
cpg	1413.69	J/mol×K	1289.96	Joback Method
cpg	1420.56	J/mol×K	1331.71	Joback Method
dvisc	0.0001493	Pa×s	649.67	Joback Method

dvisc	0.0000825	Pa×s	721.60	Joback Method
dvisc	0.0000508	Pa×s	793.53	Joback Method
dvisc	0.0000339	Pa×s	865.45	Joback Method
dvisc	0.0000241	Pa×s	937.38	Joback Method
dvisc	0.0000179	Pa×s	1009.31	Joback Method
dvisc	0.0000139	Pa×s	1081.24	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=U380620&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