Sebacic acid, 2,3-dichlorophenyl octyl ester

Inchi: InChI=1S/C24H36Cl2O4/c1-2-3-4-5-10-13-19-29-22(27)17-11-8-6-7-9-12-18-23(28)30-21
InchiKey: VZJQEVLDZGGDAF-UHFFFAOYSA-N
Formula: C24H36Cl2O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 459.45

Physical Properties

Property code	Value	Unit	Source
gf	-247.35	kJ/mol	Joback Method
hf	-846.18	kJ/mol	Joback Method
hfus	65.15	kJ/mol	Joback Method
hvap	99.70	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.923		Crippen Method
mcvol	364.620	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	1012.60	K	Joback Method
tc	1239.97	K	Joback Method
tf	615.86	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.66	J/mol×K	1012.60	Joback Method
cpg	1228.05	J/mol×K	1202.08	Joback Method
cpg	1219.16	J/mol×K	1164.18	Joback Method
cpg	1208.93	J/mol×K	1126.29	Joback Method
cpg	1197.29	J/mol×K	1088.39	Joback Method
cpg	1184.22	J/mol×K	1050.50	Joback Method
cpg	1235.63	J/mol×K	1239.97	Joback Method
dvisc	0.0000223	Pa×s	1012.60	Joback Method

dvisc	0.0000286	Pa×s	946.48	Joback Method
dvisc	0.0000380	Pa×s	880.35	Joback Method
dvisc	0.0000528	Pa×s	814.23	Joback Method
dvisc	0.0000779	Pa×s	748.11	Joback Method
dvisc	0.0001239	Pa×s	681.98	Joback Method
dvisc	0.0002177	Pa×s	615.86	Joback Method

Sources

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=U354947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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