Sebacic acid, di(2,5-dichlorophenyl) ester

Inchi: InChI=1S/C22H22Cl4O4/c23-15-9-11-17(25)19(13-15)29-21(27)7-5-3-1-2-4-6-8-22(28)30
InchiKey: ODLMEMDNQHMKKA-UHFFFAOYSA-N
Formula: C22H22Cl4O4
SMILES: O=C(CCCCCCCCC(=O)Oc1cc(Cl)ccc1Cl)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 492.22

Physical Properties

Property code	Value	Unit	Source
gf	-194.90	kJ/mol	Joback Method
hf	-622.79	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	107.62	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	7.932		Crippen Method
mcvol	337.160	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	3563.00		NIST Webbook
rinpol	3563.00		NIST Webbook
tb	1078.34	K	Joback Method
tc	1323.43	K	Joback Method
tf	704.62	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.58	J/mol×K	1078.34	Joback Method
cpg	982.06	J/mol×K	1119.19	Joback Method
cpg	989.14	J/mol×K	1160.04	Joback Method
cpg	994.87	J/mol×K	1200.88	Joback Method
cpg	999.29	J/mol×K	1241.73	Joback Method
cpg	1002.44	J/mol×K	1282.58	Joback Method
cpg	1004.38	J/mol×K	1323.43	Joback Method
dvisc	0.0001418	Pa×s	704.62	Joback Method

dvisc	0.0000930	Pa×s	766.91	Joback Method
dvisc	0.0000649	Pa×s	829.19	Joback Method
dvisc	0.0000477	Pa×s	891.48	Joback Method
dvisc	0.0000364	Pa×s	953.77	Joback Method
dvisc	0.0000288	Pa×s	1016.05	Joback Method
dvisc	0.0000234	Pa×s	1078.34	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=U355099&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