Sebacic acid, 2,6-dichlorophenyl hexyl ester

Inchi: InChI=1S/C22H32Cl2O4/c1-2-3-4-11-17-27-20(25)15-9-7-5-6-8-10-16-21(26)28-22-18(23
InchiKey: FRDCPFFNRAFUOE-UHFFFAOYSA-N
Formula: C22H32Cl2O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 431.39

Physical Properties

Property code	Value	Unit	Source
gf	-264.19	kJ/mol	Joback Method
hf	-804.90	kJ/mol	Joback Method
hfus	59.97	kJ/mol	Joback Method
hvap	95.25	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.143		Crippen Method
mcvol	336.440	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	3098.00		NIST Webbook
tb	966.84	K	Joback Method
tc	1184.56	K	Joback Method
tf	593.32	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.35	J/mol×K	966.84	Joback Method
cpg	1062.47	J/mol×K	1003.13	Joback Method
cpg	1075.27	J/mol×K	1039.41	Joback Method
cpg	1086.79	J/mol×K	1075.70	Joback Method
cpg	1097.05	J/mol×K	1111.99	Joback Method
cpg	1106.10	J/mol×K	1148.27	Joback Method
cpg	1113.96	J/mol×K	1184.56	Joback Method
dvisc	0.0002763	Pa×s	593.32	Joback Method
dvisc	0.0001606	Pa×s	655.57	Joback Method

dvisc	0.0001025	Pa×s	717.83	Joback Method
dvisc	0.0000703	Pa×s	780.08	Joback Method
dvisc	0.0000510	Pa×s	842.33	Joback Method
dvisc	0.0000386	Pa×s	904.59	Joback Method
dvisc	0.0000304	Pa×s	966.84	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=U354877&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