Sebacic acid, 2,2-dichloroethyl dodecyl ester

Inchi: InChI=1S/C24H44Cl2O4/c1-2-3-4-5-6-7-8-11-14-17-20-29-23(27)18-15-12-9-10-13-16-19
InchiKey: CGTCDVSYBLBBKI-UHFFFAOYSA-N
Formula: C24H44Cl2O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 467.51

Physical Properties

Property code	Value	Unit	Source
gf	-342.94	kJ/mol	Joback Method
hf	-1065.05	kJ/mol	Joback Method
hfus	68.36	kJ/mol	Joback Method
hvap	95.71	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.918		Crippen Method
mcvol	388.380	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
rinpol	3145.00		NIST Webbook
tb	975.52	K	Joback Method
tc	1199.01	K	Joback Method
tf	549.40	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.51	J/mol×K	975.52	Joback Method
cpg	1295.68	J/mol×K	1012.77	Joback Method
cpg	1312.26	J/mol×K	1050.02	Joback Method
cpg	1327.33	J/mol×K	1087.27	Joback Method
cpg	1340.92	J/mol×K	1124.52	Joback Method
cpg	1353.08	J/mol×K	1161.76	Joback Method
cpg	1363.88	J/mol×K	1199.01	Joback Method
dvisc	0.0003509	Pa×s	549.40	Joback Method
dvisc	0.0001627	Pa×s	620.42	Joback Method

dvisc	0.0000884	Pa×s	691.44	Joback Method
dvisc	0.0000538	Pa×s	762.46	Joback Method
dvisc	0.0000356	Pa×s	833.48	Joback Method
dvisc	0.0000252	Pa×s	904.50	Joback Method
dvisc	0.0000187	Pa×s	975.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355475&Units=SI
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

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

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