Sebacic acid, di(2,3-dichlorobenzyl) ester

Inchi: InChI=1S/C24H26Cl4O4/c25-19-11-7-9-17(23(19)27)15-31-21(29)13-5-3-1-2-4-6-14-22(3
InchiKey: ZVJHCOYZRNVBCX-UHFFFAOYSA-N
Formula: C24H26Cl4O4
SMILES: O=C(CCCCCCCCC(=O)OCc1cccc(Cl)c1Cl)OCc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 520.27

Physical Properties

Property code	Value	Unit	Source
gf	-178.06	kJ/mol	Joback Method
hf	-664.07	kJ/mol	Joback Method
hfus	66.80	kJ/mol	Joback Method
hvap	112.07	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.208		Crippen Method
mcvol	365.340	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	3663.00		NIST Webbook
rinpol	3663.00		NIST Webbook
tb	1124.10	K	Joback Method
tc	1376.29	K	Joback Method
tf	727.16	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.07	J/mol×K	1124.10	Joback Method
cpg	1099.61	J/mol×K	1166.13	Joback Method
cpg	1106.64	J/mol×K	1208.16	Joback Method
cpg	1112.22	J/mol×K	1250.20	Joback Method
cpg	1116.39	J/mol×K	1292.23	Joback Method
cpg	1119.23	J/mol×K	1334.26	Joback Method
cpg	1120.79	J/mol×K	1376.29	Joback Method
dvisc	0.0001110	Pa×s	727.16	Joback Method

dvisc	0.0000714	Pa×s	793.32	Joback Method
dvisc	0.0000491	Pa×s	859.47	Joback Method
dvisc	0.0000356	Pa×s	925.63	Joback Method
dvisc	0.0000270	Pa×s	991.79	Joback Method
dvisc	0.0000212	Pa×s	1057.94	Joback Method
dvisc	0.0000171	Pa×s	1124.10	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=U380609&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