Sebacic acid, di(2,4-dichlorophenethyl) ester

Inchi: InChI=1S/C26H30Cl4O4/c27-21-11-9-19(23(29)17-21)13-15-33-25(31)7-5-3-1-2-4-6-8-26
InchiKey: ZLXBIQPCBGGTBL-UHFFFAOYSA-N
Formula: C26H30Cl4O4
SMILES: O=C(CCCCCCCCC(=O)OCCc1ccc(Cl)cc1Cl)OCCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 548.33

Physical Properties

Property code	Value	Unit	Source
gf	-161.22	kJ/mol	Joback Method
hf	-705.35	kJ/mol	Joback Method
hfus	71.98	kJ/mol	Joback Method
hvap	116.52	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.293		Crippen Method
mcvol	393.520	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	3918.00		NIST Webbook
tb	1169.86	K	Joback Method
tc	1433.91	K	Joback Method
tf	749.70	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.96	J/mol×K	1169.86	Joback Method
cpg	1218.56	J/mol×K	1213.87	Joback Method
cpg	1225.48	J/mol×K	1257.88	Joback Method
cpg	1230.81	J/mol×K	1301.89	Joback Method
cpg	1234.63	J/mol×K	1345.90	Joback Method
cpg	1237.02	J/mol×K	1389.90	Joback Method
cpg	1238.06	J/mol×K	1433.91	Joback Method
dvisc	0.0000862	Pa×s	749.70	Joback Method
dvisc	0.0000544	Pa×s	819.73	Joback Method

dvisc	0.0000369	Pa×s	889.75	Joback Method
dvisc	0.0000265	Pa×s	959.78	Joback Method
dvisc	0.0000199	Pa×s	1029.81	Joback Method
dvisc	0.0000155	Pa×s	1099.83	Joback Method
dvisc	0.0000124	Pa×s	1169.86	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=U416825&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