Sebacic acid, di(4-chloro-2-methylbenzyl) ester

Inchi: InChI=1S/C26H32Cl2O4/c1-19-15-23(27)13-11-21(19)17-31-25(29)9-7-5-3-4-6-8-10-26(
InchiKey: OPUIQIDDCVQAAS-UHFFFAOYSA-N
Formula: C26H32Cl2O4
SMILES: Cc1cc(Cl)ccc1COC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)cc1C
Mol. weight [g/mol]: 479.44

Physical Properties

Property code	Value	Unit	Source
gf	-137.36	kJ/mol	Joback Method
hf	-673.87	kJ/mol	Joback Method
hfus	63.59	kJ/mol	Joback Method
hvap	107.75	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.518		Crippen Method
mcvol	369.040	ml/mol	McGowan Method
pc	1044.62	kPa	Joback Method
rinpol	3416.00		NIST Webbook
rinpol	3416.00		NIST Webbook
tb	1095.00	K	Joback Method
tc	1340.59	K	Joback Method
tf	689.86	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1175.92	J/mol×K	1095.00	Joback Method
cpg	1216.57	J/mol×K	1299.66	Joback Method
cpg	1211.49	J/mol×K	1258.72	Joback Method
cpg	1204.94	J/mol×K	1217.79	Joback Method
cpg	1196.87	J/mol×K	1176.86	Joback Method
cpg	1187.21	J/mol×K	1135.93	Joback Method
cpg	1220.25	J/mol×K	1340.59	Joback Method
dvisc	0.0000181	Pa×s	1095.00	Joback Method

dvisc	0.0000226	Pa×s	1027.48	Joback Method
dvisc	0.0000291	Pa×s	959.95	Joback Method
dvisc	0.0000390	Pa×s	892.43	Joback Method
dvisc	0.0000548	Pa×s	824.91	Joback Method
dvisc	0.0000817	Pa×s	757.38	Joback Method
dvisc	0.0001318	Pa×s	689.86	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=U380593&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