

Sebacic acid, di(4-chlorophenethyl) ester

Inchi: InChI=1S/C26H32Cl2O4/c27-23-13-9-21(10-14-23)17-19-31-25(29)7-5-3-1-2-4-6-8-26(30)
InchiKey: JKVVYHNRRWBTD-UHFFFAOYSA-N
Formula: C26H32Cl2O4
SMILES: O=C(CCCCCCCC(=O)OCCc1ccc(Cl)cc1)OCCc1ccc(Cl)cc1
Mol. weight [g/mol]: 479.44

Physical Properties

Property code	Value	Unit	Source
gf	-118.10	kJ/mol	Joback Method
hf	-650.93	kJ/mol	Joback Method
hfus	64.37	kJ/mol	Joback Method
hvap	106.43	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.986		Crippen Method
mvol	369.040	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1535.00		NIST Webbook
tb	1085.04	K	Joback Method
tc	1328.40	K	Joback Method
tf	664.82	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.15	J/molxK	1085.04	Joback Method
cpg	1190.97	J/molxK	1125.60	Joback Method
cpg	1201.27	J/molxK	1166.16	Joback Method
cpg	1210.13	J/molxK	1206.72	Joback Method
cpg	1217.63	J/molxK	1247.28	Joback Method
cpg	1223.85	J/molxK	1287.84	Joback Method
cpg	1228.86	J/molxK	1328.40	Joback Method
dvisc	0.0001559	Paxs	664.82	Joback Method

dvisc	0.0000904	Paxs	734.86	Joback Method
dvisc	0.0000576	Paxs	804.89	Joback Method
dvisc	0.0000395	Paxs	874.93	Joback Method
dvisc	0.0000286	Paxs	944.97	Joback Method
dvisc	0.0000217	Paxs	1015.00	Joback Method
dvisc	0.0000170	Paxs	1085.04	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=U416259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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