Pimelic acid, di(4-chlorobenzyl) ester

Inchi: InChI=1S/C21H22Cl2O4/c22-18-10-6-16(7-11-18)14-26-20(24)4-2-1-3-5-21(25)27-15-17
InchiKey: MNHDDFFWEMRITG-UHFFFAOYSA-N
Formula: C21H22Cl2O4
SMILES: O=C(CCCCCC(=O)OCc1ccc(Cl)cc1)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 409.30

Physical Properties

Property code	Value	Unit	Source
gf	-160.20	kJ/mol	Joback Method
hf	-547.73	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	95.30	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	5.731		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	3114.00		NIST Webbook
rinpol	3114.00		NIST Webbook
tb	970.64	K	Joback Method
tc	1202.13	K	Joback Method
tf	608.47	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.37	J/mol×K	970.64	Joback Method
cpg	927.02	J/mol×K	1163.55	Joback Method
cpg	920.50	J/mol×K	1124.96	Joback Method
cpg	912.82	J/mol×K	1086.38	Joback Method
cpg	903.93	J/mol×K	1047.80	Joback Method
cpg	893.80	J/mol×K	1009.22	Joback Method
cpg	932.44	J/mol×K	1202.13	Joback Method
dvisc	0.0000366	Pa×s	970.64	Joback Method

dvisc	0.0000459	Pa×s	910.28	Joback Method
dvisc	0.0000595	Pa×s	849.92	Joback Method
dvisc	0.0000803	Pa×s	789.56	Joback Method
dvisc	0.0001139	Pa×s	729.19	Joback Method
dvisc	0.0001721	Pa×s	668.83	Joback Method
dvisc	0.0002820	Pa×s	608.47	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=U406803&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