Pimelic acid, 3,5-dichlorobenzyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C20H28Cl2O4/c1-14(2)9-15(3)26-20(24)8-6-4-5-7-19(23)25-13-16-10-17(21)12

InchiKey: OPJIYCVNEVAADW-UHFFFAOYSA-N

Formula: C20H28Cl2O4

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)OCc1cc(Cl)cc(Cl)c1

Mol. weight [g/mol]: 403.34

Physical Properties

Property code	Value	Unit	Source
gf	-285.91	kJ/mol	Joback Method
hf	-774.18	kJ/mol	Joback Method
hfus	47.74	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.965		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	920.20	K	Joback Method
tc	1134.82	K	Joback Method
tf	540.78	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.10	J/mol×K	920.20	Joback Method
cpg	943.91	J/mol×K	955.97	Joback Method
cpg	956.47	J/mol×K	991.74	Joback Method
cpg	967.81	J/mol×K	1027.51	Joback Method
cpg	977.96	J/mol×K	1063.28	Joback Method
cpg	986.95	J/mol×K	1099.05	Joback Method
cpg	994.79	J/mol×K	1134.82	Joback Method
dvisc	0.0004163	Pa×s	540.78	Joback Method

dvisc	0.0002207	Pa×s	604.02	Joback Method
dvisc	0.0001319	Pa×s	667.25	Joback Method
dvisc	0.0000862	Pa×s	730.49	Joback Method
dvisc	0.0000603	Pa×s	793.73	Joback Method
dvisc	0.0000444	Pa×s	856.96	Joback Method
dvisc	0.0000342	Pa×s	920.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406685&Units=SI
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

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