Pimelic acid, 3,4-dichlorophenyl heptyl ester

Inchi: InChI=1S/C20H28Cl2O4/c1-2-3-4-5-9-14-25-19(23)10-7-6-8-11-20(24)26-16-12-13-17(21
InchiKey: GOXAGDANQUSPSK-UHFFFAOYSA-N
Formula: C20H28Cl2O4
SMILES: CCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 403.34

Physical Properties

Property code	Value	Unit	Source
gf	-281.03	kJ/mol	Joback Method
hf	-763.62	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.363		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	2777.00		NIST Webbook
rinpol	2777.00		NIST Webbook
tb	921.08	K	Joback Method
tc	1133.06	K	Joback Method
tf	570.78	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.13	J/mol×K	921.08	Joback Method
cpg	986.04	J/mol×K	1097.73	Joback Method
cpg	976.94	J/mol×K	1062.40	Joback Method
cpg	966.72	J/mol×K	1027.07	Joback Method
cpg	955.36	J/mol×K	991.74	Joback Method
cpg	942.84	J/mol×K	956.41	Joback Method
cpg	994.05	J/mol×K	1133.06	Joback Method
dvisc	0.0000410	Pa×s	921.08	Joback Method

dvisc	0.0000519	Pa×s	862.70	Joback Method
dvisc	0.0000679	Pa×s	804.31	Joback Method
dvisc	0.0000928	Pa×s	745.93	Joback Method
dvisc	0.0001336	Pa×s	687.55	Joback Method
dvisc	0.0002059	Pa×s	629.16	Joback Method
dvisc	0.0003466	Pa×s	570.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416734&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