Pimelic acid, 3,4-dichlorophenyl propyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-2-10-21-15(19)6-4-3-5-7-16(20)22-12-8-9-13(17)14(18)11-12
InchiKey: GEGAXXHQGULGKI-UHFFFAOYSA-N
Formula: C16H20Cl2O4
SMILES: CCCOC(=O)CCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-314.71	kJ/mol	Joback Method
hf	-681.06	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.803		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	829.56	K	Joback Method
tc	1039.86	K	Joback Method
tf	525.70	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.88	J/mol×K	829.56	Joback Method
cpg	711.67	J/mol×K	864.61	Joback Method
cpg	723.45	J/mol×K	899.66	Joback Method
cpg	734.25	J/mol×K	934.71	Joback Method
cpg	744.06	J/mol×K	969.76	Joback Method
cpg	752.91	J/mol×K	1004.81	Joback Method
cpg	760.81	J/mol×K	1039.86	Joback Method
dvisc	0.0005229	Pa×s	525.70	Joback Method

dvisc	0.0003260	Pa×s	576.34	Joback Method
dvisc	0.0002193	Pa×s	626.99	Joback Method
dvisc	0.0001566	Pa×s	677.63	Joback Method
dvisc	0.0001171	Pa×s	728.27	Joback Method
dvisc	0.0000910	Pa×s	778.92	Joback Method
dvisc	0.0000729	Pa×s	829.56	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=U416728&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

Latest version available from:
https://www.chemeo.com/cid/125-062-4/Pimelic-acid-3-4-dichlorophenyl-propyl-ester.pdf
Generated by Cheméo on 2024-04-30 00:08:24.016291609 +0000 UTC m=+16724952.936868924.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.