

Pimelic acid, di(3-chlorophenyl) ester

Inchi: InChI=1S/C19H18Cl2O4/c20-14-6-4-8-16(12-14)24-18(22)10-2-1-3-11-19(23)25-17-9-5-7
InchiKey: YAJQIDUZNQNEIL-UHFFFAOYSA-N
Formula: C19H18Cl2O4
SMILES: O=C(CCCCCC(=O)Oc1cccc(Cl)c1)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 381.25

Physical Properties

Property code	Value	Unit	Source
gf	-177.04	kJ/mol	Joback Method
hf	-506.45	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.455		Crippen Method
mvol	270.410	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2270.00		NIST Webbook
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tb	924.88	K	Joback Method
tc	1158.00	K	Joback Method
tf	585.93	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.42	J/molxK	924.88	Joback Method
cpg	778.65	J/molxK	963.73	Joback Method
cpg	788.63	J/molxK	1002.59	Joback Method
cpg	797.41	J/molxK	1041.44	Joback Method
cpg	805.02	J/molxK	1080.29	Joback Method
cpg	811.51	J/molxK	1119.14	Joback Method
cpg	816.89	J/molxK	1158.00	Joback Method
dvisc	0.0003501	Paxs	585.93	Joback Method

dvisc	0.0002184	Paxs	642.42	Joback Method
dvisc	0.0001471	Paxs	698.91	Joback Method
dvisc	0.0001051	Paxs	755.40	Joback Method
dvisc	0.0000787	Paxs	811.90	Joback Method
dvisc	0.0000611	Paxs	868.39	Joback Method
dvisc	0.0000490	Paxs	924.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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