

Pimelic acid, 3,4-dichlorophenyl hexyl ester

Inchi:	InChI=1S/C19H26Cl2O4/c1-2-3-4-8-13-24-18(22)9-6-5-7-10-19(23)25-15-11-12-16(20)17
InchiKey:	OKSAPCCMQCNOAM-UHFFFAOYSA-N
Formula:	C19H26Cl2O4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	389.31

Physical Properties

Property code	Value	Unit	Source
gf	-289.45	kJ/mol	Joback Method
hf	-742.98	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.973		Crippen Method
mvol	294.170	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	898.20	K	Joback Method
tc	1108.62	K	Joback Method
tf	559.51	K	Joback Method
vc	1.137	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.45	J/molxK	898.20	Joback Method
cpg	926.82	J/molxK	1073.55	Joback Method
cpg	917.74	J/molxK	1038.48	Joback Method
cpg	907.58	J/molxK	1003.41	Joback Method
cpg	896.32	J/molxK	968.34	Joback Method
cpg	883.95	J/molxK	933.27	Joback Method
cpg	934.86	J/molxK	1108.62	Joback Method
dvisc	0.0000475	Paxs	898.20	Joback Method

dvisc	0.0000599	Paxs	841.75	Joback Method
dvisc	0.0000781	Paxs	785.30	Joback Method
dvisc	0.0001062	Paxs	728.86	Joback Method
dvisc	0.0001519	Paxs	672.41	Joback Method
dvisc	0.0002321	Paxs	615.96	Joback Method
dvisc	0.0003863	Paxs	559.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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