

Pimelic acid, 3-chlorophenyl isobutyl ester

Inchi:	InChI=1S/C17H23ClO4/c1-13(2)12-21-16(19)9-4-3-5-10-17(20)22-15-8-6-7-14(18)11-15
InchiKey:	QPVOOFOVRGLNDL-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	CC(C)COC(=O)CCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-287.17	kJ/mol	Joback Method
hf	-679.77	kJ/mol	Joback Method
hfus	39.69	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.395		Crippen Method
mvol	253.750	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2356.00		NIST Webbook
rinpol	2356.00		NIST Webbook
tb	809.59	K	Joback Method
tc	1016.62	K	Joback Method
tf	479.53	K	Joback Method
vc	0.971	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.89	J/molxK	809.59	Joback Method
cpg	793.70	J/molxK	982.11	Joback Method
cpg	783.39	J/molxK	947.61	Joback Method
cpg	772.07	J/molxK	913.10	Joback Method
cpg	759.73	J/molxK	878.60	Joback Method
cpg	746.34	J/molxK	844.09	Joback Method
cpg	803.02	J/molxK	1016.62	Joback Method
dvisc	0.0000663	Paxs	809.59	Joback Method

dvisc	0.0000857	Paxs	754.58	Joback Method
dvisc	0.0001151	Paxs	699.57	Joback Method
dvisc	0.0001628	Paxs	644.56	Joback Method
dvisc	0.0002455	Paxs	589.55	Joback Method
dvisc	0.0004031	Paxs	534.54	Joback Method
dvisc	0.0007413	Paxs	479.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416669&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
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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