

Pimelic acid, 4-chloro-3-methylphenyl isobutyl ester

Inchi:	InChI=1S/C18H25ClO4/c1-13(2)12-22-17(20)7-5-4-6-8-18(21)23-15-9-10-16(19)14(3)11-
InchiKey:	PQWUDJIDINWULW-UHFFFAOYSA-N
Formula:	C18H25ClO4
SMILES:	<chem>Cc1cc(OC(=O)CCCCC(=O)OCC(C)C)ccc1Cl</chem>
Mol. weight [g/mol]:	340.84

Physical Properties

Property code	Value	Unit	Source
gf	-288.38	kJ/mol	Joback Method
hf	-711.88	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	81.57	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.704		Crippen Method
mvol	267.840	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	837.45	K	Joback Method
tc	1044.56	K	Joback Method
tf	503.32	K	Joback Method
vc	1.026	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.01	J/molxK	837.45	Joback Method
cpg	802.59	J/molxK	871.97	Joback Method
cpg	816.08	J/molxK	906.49	Joback Method
cpg	828.48	J/molxK	941.00	Joback Method
cpg	839.81	J/molxK	975.52	Joback Method
cpg	850.09	J/molxK	1010.04	Joback Method
cpg	859.32	J/molxK	1044.56	Joback Method
dvisc	0.0005729	Paxs	503.32	Joback Method

dvisc	0.0003239	Paxs	559.01	Joback Method
dvisc	0.0002030	Paxs	614.70	Joback Method
dvisc	0.0001375	Paxs	670.38	Joback Method
dvisc	0.0000989	Paxs	726.07	Joback Method
dvisc	0.0000745	Paxs	781.76	Joback Method
dvisc	0.0000583	Paxs	837.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416682&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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