

Adipic acid, 2-chloro-5-methylphenyl isohexyl ester

Inchi:	InChI=1S/C19H27ClO4/c1-14(2)7-6-12-23-18(21)8-4-5-9-19(22)24-17-13-15(3)10-11-16
InchiKey:	HWCPTZSIRRNGL-UHFFFAOYSA-N
Formula:	C19H27ClO4
SMILES:	<chem>Cc1ccc(Cl)c(OC(=O)CCCCC(=O)OCCCC(C)C)c1</chem>
Mol. weight [g/mol]:	354.87

Physical Properties

Property code	Value	Unit	Source
gf	-279.96	kJ/mol	Joback Method
hf	-732.52	kJ/mol	Joback Method
hfus	44.48	kJ/mol	Joback Method
hvap	83.80	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.094		Crippen Method
mvol	281.930	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	2492.00		NIST Webbook
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tb	860.33	K	Joback Method
tc	1067.39	K	Joback Method
tf	514.59	K	Joback Method
vc	1.083	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.93	J/molxK	860.33	Joback Method
cpg	860.72	J/molxK	894.84	Joback Method
cpg	874.36	J/molxK	929.35	Joback Method
cpg	886.88	J/molxK	963.86	Joback Method
cpg	898.29	J/molxK	998.37	Joback Method
cpg	908.61	J/molxK	1032.88	Joback Method
cpg	917.86	J/molxK	1067.39	Joback Method
dvisc	0.0005178	Paxs	514.59	Joback Method

dvisc	0.0002892	Paxs	572.21	Joback Method
dvisc	0.0001797	Paxs	629.84	Joback Method
dvisc	0.0001209	Paxs	687.46	Joback Method
dvisc	0.0000865	Paxs	745.08	Joback Method
dvisc	0.0000650	Paxs	802.71	Joback Method
dvisc	0.0000507	Paxs	860.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353960&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

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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