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

Inchi: InChI=1S/C19H27ClO4/c1-3-4-5-8-13-23-18(21)9-6-7-10-19(22)24-17-14-15(2)11-12-16(

InchiKey: MJUGRSCFIOHGGS-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: CCCCCCOC(=O)CCCCC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-277.52	kJ/mol	Joback Method
hf	-727.24	kJ/mol	Joback Method
hfus	48.00	kJ/mol	Joback Method
hvap	84.18	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.238		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
tb	860.77	K	Joback Method
tc	1066.00	K	Joback Method
tf	529.59	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.41	J/mol×K	860.77	Joback Method
cpg	860.08	J/mol×K	894.98	Joback Method
cpg	873.64	J/mol×K	929.18	Joback Method
cpg	886.11	J/mol×K	963.39	Joback Method
cpg	897.50	J/mol×K	997.59	Joback Method
cpg	907.83	J/mol×K	1031.80	Joback Method
cpg	917.12	J/mol×K	1066.00	Joback Method
dvisc	0.0004680	Pa×s	529.59	Joback Method

dvisc	0.0002772	Pa×s	584.79	Joback Method
dvisc	0.0001797	Pa×s	639.98	Joback Method
dvisc	0.0001248	Pa×s	695.18	Joback Method
dvisc	0.0000915	Pa×s	750.38	Joback Method
dvisc	0.0000699	Pa×s	805.57	Joback Method
dvisc	0.0000554	Pa×s	860.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353961&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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