Diethylmalonic acid, 4-chloro-3-methylphenyl pentyl ester

Inchi: InChI=1S/C19H27ClO4/c1-5-8-9-12-23-17(21)19(6-2,7-3)18(22)24-15-10-11-16(20)14(4)13-15

InchiKey: FFSFBMDTHHIZGV-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-274.68	kJ/mol	Joback Method
hf	-735.99	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	82.89	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.094		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1405.90	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	857.54	K	Joback Method
tc	1068.20	K	Joback Method
tf	532.01	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.41	J/mol×K	857.54	Joback Method
cpg	861.22	J/mol×K	892.65	Joback Method
cpg	874.92	J/mol×K	927.76	Joback Method
cpg	887.53	J/mol×K	962.87	Joback Method
cpg	899.09	J/mol×K	997.98	Joback Method
cpg	909.65	J/mol×K	1033.09	Joback Method
cpg	919.23	J/mol×K	1068.20	Joback Method
dvisc	0.0004205	Pa×s	532.01	Joback Method

dvisc	0.0002419	Pa×s	586.26	Joback Method
dvisc	0.0001528	Pa×s	640.52	Joback Method
dvisc	0.0001037	Pa×s	694.77	Joback Method
dvisc	0.0000745	Pa×s	749.03	Joback Method
dvisc	0.0000559	Pa×s	803.28	Joback Method
dvisc	0.0000435	Pa×s	857.54	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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