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

Inchi: InChI=1S/C22H33ClO4/c1-5-8-9-10-11-12-15-26-20(24)22(6-2,7-3)21(25)27-18-13-14-19
InchiKey: OMLOFFCTZHOSPO-UHFFFAOYSA-N
Formula: C22H33ClO4
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-249.42	kJ/mol	Joback Method
hf	-797.91	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	89.57	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.264		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	926.18	K	Joback Method
tc	1139.21	K	Joback Method
tf	565.82	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.93	J/mol×K	926.18	Joback Method
cpg	1039.29	J/mol×K	961.69	Joback Method
cpg	1053.43	J/mol×K	997.19	Joback Method
cpg	1066.40	J/mol×K	1032.70	Joback Method
cpg	1078.24	J/mol×K	1068.20	Joback Method
cpg	1089.00	J/mol×K	1103.71	Joback Method
cpg	1098.73	J/mol×K	1139.21	Joback Method
dvisc	0.0002985	Pa×s	565.82	Joback Method

dvisc	0.0001659	Pa×s	625.88	Joback Method
dvisc	0.0001022	Pa×s	685.94	Joback Method
dvisc	0.0000681	Pa×s	746.00	Joback Method
dvisc	0.0000482	Pa×s	806.06	Joback Method
dvisc	0.0000358	Pa×s	866.12	Joback Method
dvisc	0.0000276	Pa×s	926.18	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=U369917&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