Diethylmalonic acid, 4-chlorophenyl pentyl ester

Inchi: InChI=1S/C18H25ClO4/c1-4-7-8-13-22-16(20)18(5-2,6-3)17(21)23-15-11-9-14(19)10-12-

InchiKey: DAGXMRZKXHCCNL-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-273.47	kJ/mol	Joback Method
hf	-703.88	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	80.00	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.785		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	829.68	K	Joback Method
tc	1040.23	K	Joback Method
tf	508.22	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.69	J/mol×K	829.68	Joback Method
cpg	804.40	J/mol×K	864.77	Joback Method
cpg	818.01	J/mol×K	899.86	Joback Method
cpg	830.56	J/mol×K	934.95	Joback Method
cpg	842.10	J/mol×K	970.04	Joback Method
cpg	852.66	J/mol×K	1005.13	Joback Method
cpg	862.29	J/mol×K	1040.23	Joback Method
dvisc	0.0005453	Pa×s	508.22	Joback Method

dvisc	0.0003027	Pa×s	561.80	Joback Method
dvisc	0.0001862	Pa×s	615.37	Joback Method
dvisc	0.0001238	Pa×s	668.95	Joback Method
dvisc	0.0000875	Pa×s	722.53	Joback Method
dvisc	0.0000648	Pa×s	776.10	Joback Method
dvisc	0.0000499	Pa×s	829.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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