Diethylmalonic acid, 2-chlorophenyl heptyl ester

Inchi: InChI=1S/C20H29ClO4/c1-4-7-8-9-12-15-24-18(22)20(5-2,6-3)19(23)25-17-14-11-10-13-

InchiKey: UMXHYSRMKTUUDV-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-256.63	kJ/mol	Joback Method
hf	-745.16	kJ/mol	Joback Method
hfus	43.56	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.565		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	875.44	K	Joback Method
tc	1085.28	K	Joback Method
tf	530.76	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.75	J/mol×K	875.44	Joback Method
cpg	970.18	J/mol×K	1050.31	Joback Method
cpg	959.40	J/mol×K	1015.34	Joback Method
cpg	947.61	J/mol×K	980.36	Joback Method
cpg	934.77	J/mol×K	945.39	Joback Method
cpg	920.83	J/mol×K	910.41	Joback Method
cpg	980.01	J/mol×K	1085.28	Joback Method
dvisc	0.0000369	Pa×s	875.44	Joback Method

dvisc	0.0000482	Pa×s	817.99	Joback Method
dvisc	0.0000656	Pa×s	760.55	Joback Method
dvisc	0.0000937	Pa×s	703.10	Joback Method
dvisc	0.0001427	Pa×s	645.65	Joback Method
dvisc	0.0002359	Pa×s	588.21	Joback Method
dvisc	0.0004349	Pa×s	530.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369619&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