Dimethylmalonic acid, decyl pentachlorophenyl ester

Inchi: InChI=1S/C21H27Cl5O4/c1-4-5-6-7-8-9-10-11-12-29-19(27)21(2,3)20(28)30-18-16(25)14

InchiKey: WIVDOBGEGNUACA-UHFFFAOYSA-N

Formula: C21H27Cl5O4

SMILES: CCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 520.70

Physical Properties

Property code	Value	Unit	Source
gf	-334.45	kJ/mol	Joback Method
hf	-874.64	kJ/mol	Joback Method
hfus	61.39	kJ/mol	Joback Method
hvap	106.87	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	8.569		Crippen Method
mcvol	359.070	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	3242.00		NIST Webbook
rinpol	3242.00		NIST Webbook
tb	1067.96	K	Joback Method
tc	1307.87	K	Joback Method
tf	711.79	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.20	J/mol×K	1067.96	Joback Method
cpg	1085.64	J/mol×K	1267.88	Joback Method
cpg	1080.32	J/mol×K	1227.90	Joback Method
cpg	1073.86	J/mol×K	1187.91	Joback Method
cpg	1066.22	J/mol×K	1147.93	Joback Method
cpg	1057.35	J/mol×K	1107.94	Joback Method
cpg	1089.89	J/mol×K	1307.87	Joback Method
dvisc	0.0000166	Pa×s	1067.96	Joback Method

dvisc	0.0000206	Pa×s	1008.60	Joback Method
dvisc	0.0000262	Pa×s	949.24	Joback Method
dvisc	0.0000344	Pa×s	889.88	Joback Method
dvisc	0.0000471	Pa×s	830.51	Joback Method
dvisc	0.0000676	Pa×s	771.15	Joback Method
dvisc	0.0001030	Pa×s	711.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363931&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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