Dimethylmalonic acid, nonyl pentachlorophenyl ester

Inchi: InChI=1S/C20H25Cl5O4/c1-4-5-6-7-8-9-10-11-28-18(26)20(2,3)19(27)29-17-15(24)13(22
InchiKey: XIDDLXUPAOUEPY-UHFFFAOYSA-N
Formula: C20H25Cl5O4
SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 506.68

Physical Properties

Property code	Value	Unit	Source
gf	-342.87	kJ/mol	Joback Method
hf	-854.00	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	104.64	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	8.179		Crippen Method
mcvol	344.980	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
rinpol	3142.00		NIST Webbook
rinpol	3142.00		NIST Webbook
tb	1045.08	K	Joback Method
tc	1281.33	K	Joback Method
tf	700.52	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.25	J/mol×K	1045.08	Joback Method
cpg	998.23	J/mol×K	1084.45	Joback Method
cpg	1006.99	J/mol×K	1123.83	Joback Method
cpg	1014.56	J/mol×K	1163.20	Joback Method
cpg	1021.00	J/mol×K	1202.58	Joback Method
cpg	1026.35	J/mol×K	1241.95	Joback Method
cpg	1030.65	J/mol×K	1281.33	Joback Method
dvisc	0.0001168	Pa×s	700.52	Joback Method

dvisc	0.0000774	Pa×s	757.95	Joback Method
dvisc	0.0000543	Pa×s	815.37	Joback Method
dvisc	0.0000400	Pa×s	872.80	Joback Method
dvisc	0.0000305	Pa×s	930.23	Joback Method
dvisc	0.0000241	Pa×s	987.65	Joback Method
dvisc	0.0000195	Pa×s	1045.08	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=U363930&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