Diethylmalonic acid, di(2,4,6-trichlorophenyl) ester

Inchi: InChI=1S/C19H14Cl6O4/c1-3-19(4-2,17(26)28-15-11(22)5-9(20)6-12(15)23)18(27)29-16
InchiKey: HRFJLNNHBGTQKG-UHFFFAOYSA-N
Formula: C19H14Cl6O4
SMILES: CCC(CC)(C(=O)Oc1c(Cl)cc(Cl)cc1Cl)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 519.03

Physical Properties

Property code	Value	Unit	Source
gf	-260.44	kJ/mol	Joback Method
hf	-624.04	kJ/mol	Joback Method
hfus	54.06	kJ/mol	Joback Method
hvap	109.74	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.924		Crippen Method
mcvol	319.370	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	3196.00		NIST Webbook
rinpol	3196.00		NIST Webbook
tb	1091.29	K	Joback Method
tc	1349.43	K	Joback Method
tf	758.11	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.91	J/mol×K	1091.29	Joback Method
cpg	845.06	J/mol×K	1306.40	Joback Method
cpg	843.54	J/mol×K	1263.38	Joback Method
cpg	841.02	J/mol×K	1220.36	Joback Method
cpg	837.44	J/mol×K	1177.34	Joback Method
cpg	832.76	J/mol×K	1134.31	Joback Method
cpg	845.64	J/mol×K	1349.43	Joback Method
dvisc	0.0000203	Pa×s	1091.29	Joback Method

dvisc	0.0000245	Pa×s	1035.76	Joback Method
dvisc	0.0000303	Pa×s	980.23	Joback Method
dvisc	0.0000384	Pa×s	924.70	Joback Method
dvisc	0.0000501	Pa×s	869.17	Joback Method
dvisc	0.0000678	Pa×s	813.64	Joback Method
dvisc	0.0000961	Pa×s	758.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370157&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