Diethylmalonic acid, di(2,4-dichloro-6-formylphenyl) ester

Inchi: InChI=1S/C21H16Cl4O6/c1-3-21(4-2,19(28)30-17-11(9-26)5-13(22)7-15(17)24)20(29)31
InchiKey: GLBLHWHVXXTAHP-UHFFFAOYSA-N
Formula: C21H16Cl4O6
SMILES: CCC(CC)(C(=O)Oc1c(Cl)cc(Cl)cc1C=O)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]: 506.16

Physical Properties

Property code	Value	Unit	Source
gf	-418.78	kJ/mol	Joback Method
hf	-805.00	kJ/mol	Joback Method
hfus	55.42	kJ/mol	Joback Method
hvap	118.86	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.243		Crippen Method
mcvol	326.210	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	3311.00		NIST Webbook
tb	1159.51	K	Joback Method
tc	1421.72	K	Joback Method
tf	804.81	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.13	J/mol×K	1159.51	Joback Method
cpg	910.42	J/mol×K	1203.21	Joback Method
cpg	913.40	J/mol×K	1246.91	Joback Method
cpg	915.15	J/mol×K	1290.62	Joback Method
cpg	915.73	J/mol×K	1334.32	Joback Method
cpg	915.18	J/mol×K	1378.02	Joback Method
cpg	913.57	J/mol×K	1421.72	Joback Method
dvisc	0.0001137	Pa×s	804.81	Joback Method
dvisc	0.0000802	Pa×s	863.93	Joback Method

dvisc	0.0000592	Pa×s	923.04	Joback Method
dvisc	0.0000454	Pa×s	982.16	Joback Method
dvisc	0.0000358	Pa×s	1041.28	Joback Method
dvisc	0.0000290	Pa×s	1100.39	Joback Method
dvisc	0.0000240	Pa×s	1159.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370075&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