Diethylmalonic acid, 2,4-dichloro-6-formylphenyl pentyl ester

Inchi: InChI=1S/C19H24Cl2O5/c1-4-7-8-9-25-17(23)19(5-2,6-3)18(24)26-16-13(12-22)10-14(20

InchiKey: OLURWXBBXYZAQI-UHFFFAOYSA-N

Formula: C19H24Cl2O5

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 403.30

Physical Properties

Property code	Value	Unit	Source
gf	-395.76	kJ/mol	Joback Method
hf	-848.78	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	94.66	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.251		Crippen Method
mcvol	295.740	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2492.00		NIST Webbook
tb	948.61	K	Joback Method
tc	1170.08	K	Joback Method
tf	616.45	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.83	J/mol×K	948.61	Joback Method
cpg	891.48	J/mol×K	985.52	Joback Method
cpg	902.00	J/mol×K	1022.43	Joback Method
cpg	911.43	J/mol×K	1059.35	Joback Method
cpg	919.81	J/mol×K	1096.26	Joback Method
cpg	927.17	J/mol×K	1133.17	Joback Method
cpg	933.56	J/mol×K	1170.08	Joback Method
dvisc	0.0002883	Pa×s	616.45	Joback Method
dvisc	0.0001808	Pa×s	671.81	Joback Method

dvisc	0.0001217	Pa×s	727.17	Joback Method
dvisc	0.0000867	Pa×s	782.53	Joback Method
dvisc	0.0000645	Pa×s	837.89	Joback Method
dvisc	0.0000498	Pa×s	893.25	Joback Method
dvisc	0.0000397	Pa×s	948.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370064&Units=SI

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