Dimethylmalonic acid, 2,4-dichloro-6-formylphenyl octyl ester

Inchi: InChI=1S/C20H26Cl2O5/c1-4-5-6-7-8-9-10-26-18(24)20(2,3)19(25)27-17-14(13-23)11-15

InchiKey: IXMHHWOGUWIWNY-UHFFFAOYSA-N

Formula: C20H26Cl2O5

SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 417.32

Physical Properties

Property code	Value	Unit	Source
gf	-387.34	kJ/mol	Joback Method
hf	-869.42	kJ/mol	Joback Method
hfus	49.27	kJ/mol	Joback Method
hvap	96.88	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.641		Crippen Method
mcvol	309.830	ml/mol	McGowan Method
pc	1331.01	kPa	Joback Method
rinpol	2629.00		NIST Webbook
rinpol	2629.00		NIST Webbook
tb	971.49	K	Joback Method
tc	1194.48	K	Joback Method
tf	627.72	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.13	J/mol×K	971.49	Joback Method
cpg	986.08	J/mol×K	1157.32	Joback Method
cpg	978.66	J/mol×K	1120.15	Joback Method
cpg	970.20	J/mol×K	1082.99	Joback Method
cpg	960.66	J/mol×K	1045.82	Joback Method
cpg	949.98	J/mol×K	1008.66	Joback Method
cpg	992.50	J/mol×K	1194.48	Joback Method
dvisc	0.0000340	Pa×s	971.49	Joback Method

dvisc	0.0000428	Pa×s	914.19	Joback Method
dvisc	0.0000557	Pa×s	856.90	Joback Method
dvisc	0.0000752	Pa×s	799.61	Joback Method
dvisc	0.0001062	Pa×s	742.31	Joback Method
dvisc	0.0001591	Pa×s	685.01	Joback Method
dvisc	0.0002566	Pa×s	627.72	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=U363637&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