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

Inchi: InChI=1S/C21H28Cl2O5/c1-4-5-6-7-8-9-10-11-27-19(25)21(2,3)20(26)28-18-15(14-24)12

InchiKey: VDEIBMKVQGBIPM-UHFFFAOYSA-N

Formula: C21H28Cl2O5

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

Mol. weight [g/mol]: 431.35

Physical Properties

Property code	Value	Unit	Source
gf	-378.92	kJ/mol	Joback Method
hf	-890.06	kJ/mol	Joback Method
hfus	51.86	kJ/mol	Joback Method
hvap	99.11	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.031		Crippen Method
mcvol	323.920	ml/mol	McGowan Method
pc	1242.46	kPa	Joback Method
rinpol	2730.00		NIST Webbook
tb	994.37	K	Joback Method
tc	1219.80	K	Joback Method
tf	638.99	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.03	J/mol×K	994.37	Joback Method
cpg	1045.52	J/mol×K	1182.23	Joback Method
cpg	1038.07	J/mol×K	1144.66	Joback Method
cpg	1029.55	J/mol×K	1107.09	Joback Method
cpg	1019.90	J/mol×K	1069.51	Joback Method
cpg	1009.07	J/mol×K	1031.94	Joback Method
cpg	1051.95	J/mol×K	1219.80	Joback Method
dvisc	0.0000291	Pa×s	994.37	Joback Method
dvisc	0.0000368	Pa×s	935.14	Joback Method

dvisc	0.0000480	Pa×s	875.91	Joback Method
dvisc	0.0000651	Pa×s	816.68	Joback Method
dvisc	0.0000925	Pa×s	757.45	Joback Method
dvisc	0.0001397	Pa×s	698.22	Joback Method
dvisc	0.0002277	Pa×s	638.99	Joback Method

Sources

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=U363638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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