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

Inchi: InChI=1S/C22H30Cl2O5/c1-4-7-8-9-10-11-12-28-20(26)22(5-2,6-3)21(27)29-19-16(15-25

InchiKey: GZSAGXZNKRDPRQ-UHFFFAOYSA-N

Formula: C22H30Cl2O5

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

Mol. weight [g/mol]: 445.38

Physical Properties

Property code	Value	Unit	Source
gf	-370.50	kJ/mol	Joback Method
hf	-910.70	kJ/mol	Joback Method
hfus	54.45	kJ/mol	Joback Method
hvap	101.33	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.421		Crippen Method
mcvol	338.010	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
rinpol	2779.00		NIST Webbook
rinpol	2779.00		NIST Webbook
tb	1017.25	K	Joback Method
tc	1246.09	K	Joback Method
tf	650.26	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.48	J/mol×K	1017.25	Joback Method
cpg	1105.47	J/mol×K	1207.95	Joback Method
cpg	1098.01	J/mol×K	1169.81	Joback Method
cpg	1089.43	J/mol×K	1131.67	Joback Method
cpg	1079.68	J/mol×K	1093.53	Joback Method
cpg	1068.72	J/mol×K	1055.39	Joback Method
cpg	1111.88	J/mol×K	1246.09	Joback Method
dvisc	0.0000248	Pa×s	1017.25	Joback Method

dvisc	0.0000315	Pa×s	956.09	Joback Method
dvisc	0.0000412	Pa×s	894.92	Joback Method
dvisc	0.0000562	Pa×s	833.75	Joback Method
dvisc	0.0000804	Pa×s	772.59	Joback Method
dvisc	0.0001224	Pa×s	711.42	Joback Method
dvisc	0.0002016	Pa×s	650.26	Joback Method

Sources

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=U370068&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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