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

Inchi: InChI=1S/C24H34Cl2O5/c1-4-7-8-9-10-11-12-13-14-30-22(28)24(5-2,6-3)23(29)31-21-18

InchiKey: ITWLWHQVUHDWPK-UHFFFAOYSA-N

Formula: C24H34Cl2O5

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

Mol. weight [g/mol]: 473.43

Physical Properties

Property code	Value	Unit	Source
gf	-353.66	kJ/mol	Joback Method
hf	-951.98	kJ/mol	Joback Method
hfus	59.63	kJ/mol	Joback Method
hvap	105.79	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.202		Crippen Method
mcvol	366.190	ml/mol	McGowan Method
pc	1024.00	kPa	Joback Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook
tb	1063.01	K	Joback Method
tc	1301.86	K	Joback Method
tf	672.80	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.81	J/mol×K	1063.01	Joback Method
cpg	1189.48	J/mol×K	1102.82	Joback Method
cpg	1200.75	J/mol×K	1142.63	Joback Method
cpg	1210.67	J/mol×K	1182.43	Joback Method
cpg	1219.32	J/mol×K	1222.24	Joback Method
cpg	1226.78	J/mol×K	1262.05	Joback Method
cpg	1233.10	J/mol×K	1301.86	Joback Method
dvisc	0.0001568	Pa×s	672.80	Joback Method

dvisc	0.0000933	Pa×s	737.84	Joback Method
dvisc	0.0000604	Pa×s	802.87	Joback Method
dvisc	0.0000417	Pa×s	867.90	Joback Method
dvisc	0.0000303	Pa×s	932.94	Joback Method
dvisc	0.0000230	Pa×s	997.97	Joback Method
dvisc	0.0000180	Pa×s	1063.01	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=U370070&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