Diethylmalonic acid, decyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C23H33Cl3O4/c1-4-7-8-9-10-11-12-13-14-29-21(27)23(5-2,6-3)22(28)30-20-18

InchiKey: YLMMQDQXESHLJV-UHFFFAOYSA-N

Formula: C23H33Cl3O4

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 479.87

Physical Properties

Property code	Value	Unit	Source
gf	-274.49	kJ/mol	Joback Method
hf	-861.50	kJ/mol	Joback Method
hfus	58.95	kJ/mol	Joback Method
hvap	101.22	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	8.043		Crippen Method
mcvol	362.770	ml/mol	McGowan Method
pc	1014.24	kPa	Joback Method
rinpol	2961.00		NIST Webbook
tb	1028.90	K	Joback Method
tc	1259.85	K	Joback Method
tf	649.45	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.37	J/mol×K	1028.90	Joback Method
cpg	1143.54	J/mol×K	1067.39	Joback Method
cpg	1155.40	J/mol×K	1105.88	Joback Method
cpg	1166.02	J/mol×K	1144.37	Joback Method
cpg	1175.46	J/mol×K	1182.86	Joback Method
cpg	1183.78	J/mol×K	1221.35	Joback Method
cpg	1191.06	J/mol×K	1259.85	Joback Method
dvisc	0.0001486	Pa×s	649.45	Joback Method
dvisc	0.0000878	Pa×s	712.69	Joback Method

dvisc	0.0000566	Pa×s	775.93	Joback Method
dvisc	0.0000389	Pa×s	839.17	Joback Method
dvisc	0.0000282	Pa×s	902.42	Joback Method
dvisc	0.0000214	Pa×s	965.66	Joback Method
dvisc	0.0000167	Pa×s	1028.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370154&Units=SI
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

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