Diethylmalonic acid, nonyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C22H31Cl3O4/c1-4-7-8-9-10-11-12-15-28-20(26)22(5-2,6-3)21(27)29-19-17(24

InchiKey: UCXUWUFPNMMSSP-UHFFFAOYSA-N

Formula: C22H31Cl3O4

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)ccc(Cl)c1Cl

Mol. weight [g/mol]: 465.84

Physical Properties

Property code	Value	Unit	Source
gf	-282.91	kJ/mol	Joback Method
hf	-840.86	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	99.00	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.652		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2902.00		NIST Webbook
tb	1006.02	K	Joback Method
tc	1232.99	K	Joback Method
tf	638.18	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.18	J/mol×K	1006.02	Joback Method
cpg	1122.99	J/mol×K	1195.16	Joback Method
cpg	1114.70	J/mol×K	1157.33	Joback Method
cpg	1105.33	J/mol×K	1119.51	Joback Method
cpg	1094.83	J/mol×K	1081.68	Joback Method
cpg	1083.13	J/mol×K	1043.85	Joback Method
cpg	1130.26	J/mol×K	1232.99	Joback Method
dvisc	0.0000196	Pa×s	1006.02	Joback Method
dvisc	0.0000250	Pa×s	944.71	Joback Method

dvisc	0.0000330	Pa×s	883.41	Joback Method
dvisc	0.0000452	Pa×s	822.10	Joback Method
dvisc	0.0000654	Pa×s	760.79	Joback Method
dvisc	0.0001007	Pa×s	699.49	Joback Method
dvisc	0.0001686	Pa×s	638.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370289&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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