Diethylmalonic acid, 2,3-dichlorophenyl nonyl ester

Inchi: InChI=1S/C22H32Cl2O4/c1-4-7-8-9-10-11-12-16-27-20(25)22(5-2,6-3)21(26)28-18-15-13

InchiKey: BLTILWPQVYPUCO-UHFFFAOYSA-N

Formula: C22H32Cl2O4

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 431.39

Physical Properties

Property code	Value	Unit	Source
gf	-261.35	kJ/mol	Joback Method
hf	-813.65	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	93.95	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.999		Crippen Method
mcvol	336.440	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2713.00		NIST Webbook
tb	963.61	K	Joback Method
tc	1182.85	K	Joback Method
tf	595.74	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.62	J/mol×K	963.61	Joback Method
cpg	1107.97	J/mol×K	1146.31	Joback Method
cpg	1098.32	J/mol×K	1109.77	Joback Method
cpg	1087.62	J/mol×K	1073.23	Joback Method
cpg	1075.81	J/mol×K	1036.69	Joback Method
cpg	1062.83	J/mol×K	1000.15	Joback Method
cpg	1116.62	J/mol×K	1182.85	Joback Method
dvisc	0.0000231	Pa×s	963.61	Joback Method
dvisc	0.0000299	Pa×s	902.30	Joback Method

dvisc	0.0000400	Pa×s	840.99	Joback Method
dvisc	0.0000562	Pa×s	779.67	Joback Method
dvisc	0.0000837	Pa×s	718.36	Joback Method
dvisc	0.0001342	Pa×s	657.05	Joback Method
dvisc	0.0002370	Pa×s	595.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370037&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