Diethylmalonic acid, 4-chlorophenyl nonyl ester

Inchi: InChI=1S/C22H33ClO4/c1-4-7-8-9-10-11-12-17-26-20(24)22(5-2,6-3)21(25)27-19-15-13-

InchiKey: NTILLDNQKHDOIY-UHFFFAOYSA-N

Formula: C22H33ClO4

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-239.79	kJ/mol	Joback Method
hf	-786.44	kJ/mol	Joback Method
hfus	48.74	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.346		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2514.00		NIST Webbook
rinpol	2514.00		NIST Webbook
tb	921.20	K	Joback Method
tc	1133.31	K	Joback Method
tf	553.30	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.74	J/mol×K	921.20	Joback Method
cpg	1040.19	J/mol×K	956.55	Joback Method
cpg	1054.44	J/mol×K	991.90	Joback Method
cpg	1067.54	J/mol×K	1027.26	Joback Method
cpg	1079.53	J/mol×K	1062.61	Joback Method
cpg	1090.48	J/mol×K	1097.96	Joback Method
cpg	1100.43	J/mol×K	1133.31	Joback Method
dvisc	0.0003423	Pa×s	553.30	Joback Method

dvisc	0.0001817	Pa×s	614.62	Joback Method
dvisc	0.0001082	Pa×s	675.93	Joback Method
dvisc	0.0000702	Pa×s	737.25	Joback Method
dvisc	0.0000487	Pa×s	798.57	Joback Method
dvisc	0.0000356	Pa×s	859.88	Joback Method
dvisc	0.0000271	Pa×s	921.20	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=U369899&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

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