Diethylmalonic acid, 4-chlorophenyl undecyl ester

Inchi: InChI=1S/C24H37ClO4/c1-4-7-8-9-10-11-12-13-14-19-28-22(26)24(5-2,6-3)23(27)29-21-

InchiKey: OQVBWZDFNKBGAY-UHFFFAOYSA-N

Formula: C24H37ClO4

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

Mol. weight [g/mol]: 425.00

Physical Properties

Property code	Value	Unit	Source
gf	-222.95	kJ/mol	Joback Method
hf	-827.72	kJ/mol	Joback Method
hfus	53.92	kJ/mol	Joback Method
hvap	93.36	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	7.126		Crippen Method
mcvol	352.380	ml/mol	McGowan Method
pc	1019.43	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	966.96	K	Joback Method
tc	1184.75	K	Joback Method
tf	575.84	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.21	J/mol×K	966.96	Joback Method
cpg	1162.09	J/mol×K	1003.26	Joback Method
cpg	1176.69	J/mol×K	1039.56	Joback Method
cpg	1190.05	J/mol×K	1075.86	Joback Method
cpg	1202.25	J/mol×K	1112.15	Joback Method
cpg	1213.35	J/mol×K	1148.45	Joback Method
cpg	1223.41	J/mol×K	1184.75	Joback Method
dvisc	0.0002663	Pa×s	575.84	Joback Method

dvisc	0.0001385	Pa×s	641.03	Joback Method
dvisc	0.0000813	Pa×s	706.21	Joback Method
dvisc	0.0000522	Pa×s	771.40	Joback Method
dvisc	0.0000359	Pa×s	836.59	Joback Method
dvisc	0.0000261	Pa×s	901.77	Joback Method
dvisc	0.0000198	Pa×s	966.96	Joback Method

Sources

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=U369901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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