Diethylmalonic acid, 4-chloro-2-methylphenyl undecyl ester

Inchi: InChI=1S/C25H39ClO4/c1-5-8-9-10-11-12-13-14-15-18-29-23(27)25(6-2,7-3)24(28)30-22

InchiKey: ACGBXOQRXVNIBV-UHFFFAOYSA-N

Formula: C25H39ClO4

SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 439.03

Physical Properties

Property code	Value	Unit	Source
gf	-224.16	kJ/mol	Joback Method
hf	-859.83	kJ/mol	Joback Method
hfus	56.13	kJ/mol	Joback Method
hvap	96.24	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.434		Crippen Method
mcvol	366.470	ml/mol	McGowan Method
pc	950.84	kPa	Joback Method
rinpol	2848.00		NIST Webbook
tb	994.82	K	Joback Method
tc	1217.98	K	Joback Method
tf	599.63	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.95	J/mol×K	994.82	Joback Method
cpg	1222.98	J/mol×K	1032.01	Joback Method
cpg	1237.62	J/mol×K	1069.21	Joback Method
cpg	1250.94	J/mol×K	1106.40	Joback Method
cpg	1263.02	J/mol×K	1143.59	Joback Method
cpg	1273.91	J/mol×K	1180.78	Joback Method
cpg	1283.68	J/mol×K	1217.98	Joback Method
dvisc	0.0002061	Pa×s	599.63	Joback Method
dvisc	0.0001111	Pa×s	665.50	Joback Method

dvisc	0.0000670	Pa×s	731.36	Joback Method
dvisc	0.0000439	Pa×s	797.23	Joback Method
dvisc	0.0000307	Pa×s	863.09	Joback Method
dvisc	0.0000225	Pa×s	928.95	Joback Method
dvisc	0.0000173	Pa×s	994.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370115&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