Diethylmalonic acid, 4-chlorophenyl pentadecyl ester

Inchi: InChI=1S/C28H45ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-23-32-26(30)28(5-2,6-3)
InchiKey: KFCVGZWXTHSGOJ-UHFFFAOYSA-N
Formula: C28H45ClO4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 481.11

Physical Properties

Property code	Value	Unit	Source
gf	-189.27	kJ/mol	Joback Method
hf	-910.28	kJ/mol	Joback Method
hfus	64.28	kJ/mol	Joback Method
hvap	102.26	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	8.686		Crippen Method
mcvol	408.740	ml/mol	McGowan Method
pc	808.91	kPa	Joback Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook
tb	1058.48	K	Joback Method
tc	1299.92	K	Joback Method
tf	620.92	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.04	J/mol×K	1058.48	Joback Method
cpg	1466.09	J/mol×K	1259.68	Joback Method
cpg	1454.61	J/mol×K	1219.44	Joback Method
cpg	1441.87	J/mol×K	1179.20	Joback Method
cpg	1427.77	J/mol×K	1138.96	Joback Method
cpg	1412.19	J/mol×K	1098.72	Joback Method
cpg	1476.43	J/mol×K	1299.92	Joback Method
dvisc	0.0000104	Pa×s	1058.48	Joback Method

dvisc	0.0000138	Pa×s	985.55	Joback Method
dvisc	0.0000192	Pa×s	912.63	Joback Method
dvisc	0.0000283	Pa×s	839.70	Joback Method
dvisc	0.0000449	Pa×s	766.77	Joback Method
dvisc	0.0000784	Pa×s	693.85	Joback Method
dvisc	0.0001564	Pa×s	620.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369905&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