Diethylmalonic acid, 4-chloro-3-methylphenyl dodecyl ester

Inchi: InChI=1S/C26H41ClO4/c1-5-8-9-10-11-12-13-14-15-16-19-30-24(28)26(6-2,7-3)25(29)31

InchiKey: HHGCVFVKQDLRKK-UHFFFAOYSA-N

Formula: C26H41ClO4

SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 453.05

Physical Properties

Property code	Value	Unit	Source
gf	-215.74	kJ/mol	Joback Method
hf	-880.47	kJ/mol	Joback Method
hfus	58.72	kJ/mol	Joback Method
hvap	98.47	kJ/mol	Joback Method
log10ws	-8.68		Crippen Method
logp	7.824		Crippen Method
mcvol	380.560	ml/mol	McGowan Method
pc	896.95	kPa	Joback Method
rinpol	2941.00		NIST Webbook
rinpol	2941.00		NIST Webbook
tb	1017.70	K	Joback Method
tc	1246.25	K	Joback Method
tf	610.90	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.95	J/mol×K	1017.70	Joback Method
cpg	1336.65	J/mol×K	1208.15	Joback Method
cpg	1325.72	J/mol×K	1170.06	Joback Method
cpg	1313.56	J/mol×K	1131.97	Joback Method
cpg	1300.09	J/mol×K	1093.88	Joback Method
cpg	1285.25	J/mol×K	1055.79	Joback Method
cpg	1346.43	J/mol×K	1246.25	Joback Method
dvisc	0.0000147	Pa×s	1017.70	Joback Method

dvisc	0.0000193	Pa×s	949.90	Joback Method
dvisc	0.0000263	Pa×s	882.10	Joback Method
dvisc	0.0000377	Pa×s	814.30	Joback Method
dvisc	0.0000579	Pa×s	746.50	Joback Method
dvisc	0.0000968	Pa×s	678.70	Joback Method
dvisc	0.0001813	Pa×s	610.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369921&Units=SI

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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