Diethylmalonic acid, 3-chlorobenzyl pentadecyl ester

Inchi: InChI=1S/C29H47ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-22-33-27(31)29(5-2,6-3)
InchiKey: OSOGZWNSTJXONA-UHFFFAOYSA-N
Formula: C29H47ClO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1
Mol. weight [g/mol]: 495.13

Physical Properties

Property code	Value	Unit	Source
gf	-180.85	kJ/mol	Joback Method
hf	-930.92	kJ/mol	Joback Method
hfus	66.88	kJ/mol	Joback Method
hvap	104.49	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.824		Crippen Method
mcvol	422.830	ml/mol	McGowan Method
pc	766.49	kPa	Joback Method
rinpol	3262.00		NIST Webbook
rinpol	3262.00		NIST Webbook
tb	1081.36	K	Joback Method
tc	1331.72	K	Joback Method
tf	632.19	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.25	J/mol×K	1081.36	Joback Method
cpg	1530.64	J/mol×K	1289.99	Joback Method
cpg	1519.01	J/mol×K	1248.27	Joback Method
cpg	1506.09	J/mol×K	1206.54	Joback Method
cpg	1491.73	J/mol×K	1164.81	Joback Method
cpg	1475.83	J/mol×K	1123.09	Joback Method
cpg	1541.09	J/mol×K	1331.72	Joback Method
dvisc	0.0000088	Pa×s	1081.36	Joback Method

dvisc	0.0000117	Pa×s	1006.50	Joback Method
dvisc	0.0000163	Pa×s	931.64	Joback Method
dvisc	0.0000242	Pa×s	856.77	Joback Method
dvisc	0.0000385	Pa×s	781.91	Joback Method
dvisc	0.0000677	Pa×s	707.05	Joback Method
dvisc	0.0001362	Pa×s	632.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369354&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