

Diethylmalonic acid, 2-chlorophenyl hexadecyl ester

Inchi:	InChI=1S/C29H47ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-21-24-33-27(31)29(5-2,6
InchiKey:	RKKWUSZOYDZFGU-UHFFFAOYSA-N
Formula:	C29H47ClO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl
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	-9.88		Crippen Method
logp	9.076		Crippen Method
mcvol	422.830	ml/mol	McGowan Method
pc	766.49	kPa	Joback Method
rinpol	3287.00		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/molxK	1081.36	Joback Method
cpg	1530.64	J/molxK	1289.99	Joback Method
cpg	1519.01	J/molxK	1248.27	Joback Method
cpg	1506.09	J/molxK	1206.54	Joback Method
cpg	1491.73	J/molxK	1164.81	Joback Method
cpg	1475.83	J/molxK	1123.09	Joback Method
cpg	1541.09	J/molxK	1331.72	Joback Method
dvisc	0.0000088	Paxs	1081.36	Joback Method
dvisc	0.0000117	Paxs	1006.50	Joback Method

dvisc	0.0000163	Paxs	931.64	Joback Method
dvisc	0.0000242	Paxs	856.77	Joback Method
dvisc	0.0000385	Paxs	781.91	Joback Method
dvisc	0.0000677	Paxs	707.05	Joback Method
dvisc	0.0001362	Paxs	632.19	Joback Method

Sources

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=U369626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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