

Diethylmalonic acid, 2-chlorophenyl heptadecyl ester

Inchi:	InChI=1S/C30H49ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-34-28(32)30(5
InchiKey:	FCICHOIPTPCMRR-UHFFFAOYSA-N
Formula:	C30H49ClO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	509.16

Physical Properties

Property code	Value	Unit	Source
gf	-172.43	kJ/mol	Joback Method
hf	-951.56	kJ/mol	Joback Method
hfus	69.47	kJ/mol	Joback Method
hvap	106.71	kJ/mol	Joback Method
log10ws	-10.30		Crippen Method
logp	9.466		Crippen Method
mcvol	436.920	ml/mol	McGowan Method
pc	727.31	kPa	Joback Method
rinsol	3388.00		NIST Webbook
tb	1104.24	K	Joback Method
tc	1364.90	K	Joback Method
tf	643.46	K	Joback Method
vc	1.694	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.79	J/molxK	1104.24	Joback Method
cpg	1539.86	J/molxK	1147.68	Joback Method
cpg	1556.13	J/molxK	1191.13	Joback Method
cpg	1570.77	J/molxK	1234.57	Joback Method
cpg	1583.92	J/molxK	1278.01	Joback Method
cpg	1595.72	J/molxK	1321.46	Joback Method
cpg	1606.32	J/molxK	1364.90	Joback Method
dvisc	0.0001184	Paxs	643.46	Joback Method
dvisc	0.0000584	Paxs	720.26	Joback Method

dvisc	0.0000330	Paxs	797.05	Joback Method
dvisc	0.0000206	Paxs	873.85	Joback Method
dvisc	0.0000139	Paxs	950.65	Joback Method
dvisc	0.0000099	Paxs	1027.44	Joback Method
dvisc	0.0000074	Paxs	1104.24	Joback Method

Sources

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=U369627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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