

Diethylmalonic acid, 4-chlorophenyl octadecyl ester

Inchi:	InChI=1S/C31H51ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-26-35-29(33)3
InchiKey:	KXVBGFLNXWFBFX-UHFFFAOYSA-N
Formula:	C31H51ClO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	523.19

Physical Properties

Property code	Value	Unit	Source
gf	-164.01	kJ/mol	Joback Method
hf	-972.20	kJ/mol	Joback Method
hfus	72.05	kJ/mol	Joback Method
hvap	108.94	kJ/mol	Joback Method
log10ws	-10.72		Crippen Method
logp	9.856		Crippen Method
mvol	451.010	ml/mol	McGowan Method
pc	691.07	kPa	Joback Method
rinpol	3444.00		NIST Webbook
rinpol	3444.00		NIST Webbook
tb	1127.12	K	Joback Method
tc	1399.57	K	Joback Method
tf	654.73	K	Joback Method
vc	1.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.63	J/molxK	1127.12	Joback Method
cpg	1661.34	J/molxK	1354.16	Joback Method
cpg	1649.32	J/molxK	1308.75	Joback Method
cpg	1635.92	J/molxK	1263.34	Joback Method
cpg	1620.95	J/molxK	1217.94	Joback Method
cpg	1604.25	J/molxK	1172.53	Joback Method
cpg	1672.14	J/molxK	1399.57	Joback Method
dvisc	0.0000063	Paxs	1127.12	Joback Method

dvisc	0.0000084	Paxs	1048.39	Joback Method
dvisc	0.0000118	Paxs	969.66	Joback Method
dvisc	0.0000176	Paxs	890.92	Joback Method
dvisc	0.0000282	Paxs	812.19	Joback Method
dvisc	0.0000502	Paxs	733.46	Joback Method
dvisc	0.0001027	Paxs	654.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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