

Diethylmalonic acid, 2-chlorophenyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C20H29ClO4/c1-6-11-16(14(4)5)24-18(22)20(7-2,8-3)19(23)25-17-13-10-9-12
InchiKey:	WPRTVIXEATXAFN-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CCCC(OC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl)C(C)C
Mol. weight [g/mol]:	368.89

Physical Properties

Property code	Value	Unit	Source
gf	-261.51	kJ/mol	Joback Method
hf	-755.72	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	83.68	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.420		Crippen Method
mvol	296.020	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2208.00		NIST Webbook
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tb	874.56	K	Joback Method
tc	1088.45	K	Joback Method
tf	500.76	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.78	J/molxK	874.56	Joback Method
cpg	922.11	J/molxK	910.21	Joback Method
cpg	936.21	J/molxK	945.86	Joback Method
cpg	949.16	J/molxK	981.51	Joback Method
cpg	960.99	J/molxK	1017.16	Joback Method
cpg	971.76	J/molxK	1052.80	Joback Method
cpg	981.50	J/molxK	1088.45	Joback Method
dvisc	0.0005631	Paxs	500.76	Joback Method

dvisc	0.0002657	Paxs	563.06	Joback Method
dvisc	0.0001456	Paxs	625.36	Joback Method
dvisc	0.0000890	Paxs	687.66	Joback Method
dvisc	0.0000590	Paxs	749.96	Joback Method
dvisc	0.0000417	Paxs	812.26	Joback Method
dvisc	0.0000309	Paxs	874.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369617&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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