

Diethylmalonic acid, 4-chloro-3-methylphenyl propyl ester

Inchi:	InChI=1S/C17H23ClO4/c1-5-10-21-15(19)17(6-2,7-3)16(20)22-13-8-9-14(18)12(4)11-13/
InchiKey:	XVBYKCULCPQFSC-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-291.52	kJ/mol	Joback Method
hf	-694.71	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.313		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinsol	2064.00		NIST Webbook
tb	811.78	K	Joback Method
tc	1024.45	K	Joback Method
tf	509.47	K	Joback Method
vc	0.966	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.90	J/molxK	811.78	Joback Method
cpg	746.30	J/molxK	847.22	Joback Method
cpg	759.64	J/molxK	882.67	Joback Method
cpg	771.93	J/molxK	918.11	Joback Method
cpg	783.22	J/molxK	953.56	Joback Method
cpg	793.54	J/molxK	989.00	Joback Method
cpg	802.91	J/molxK	1024.45	Joback Method
dvisc	0.0005189	Paxs	509.47	Joback Method
dvisc	0.0003060	Paxs	559.86	Joback Method

dvisc	0.0001968	Paxs	610.24	Joback Method
dvisc	0.0001355	Paxs	660.62	Joback Method
dvisc	0.0000983	Paxs	711.01	Joback Method
dvisc	0.0000744	Paxs	761.39	Joback Method
dvisc	0.0000583	Paxs	811.78	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=U369911&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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