

DDA Methyl ester

Other names:	p,p'-DDA methyl ester Methyl bis(p-chlorophenyl)acetate methyl bis(4-chlorophenyl)ethanoate
Inchi:	InChI=1S/C15H12Cl2O2/c1-19-15(18)14(10-2-6-12(16)7-3-10)11-4-8-13(17)9-5-11/h2-9,
InchiKey:	FIHLIVMWNUSLRU-UHFFFAOYSA-N
Formula:	C15H12Cl2O2
SMILES:	COC(=O)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	295.16
CAS:	5359-38-6

Physical Properties

Property code	Value	Unit	Source
gf	20.76	kJ/mol	Joback Method
hf	-184.37	kJ/mol	Joback Method
hfus	29.57	kJ/mol	Joback Method
hvap	72.40	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.298		Crippen Method
mcvol	206.610	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	756.63	K	Joback Method
tc	1005.36	K	Joback Method
tf	312.00 ± 0.20	K	NIST Webbook
vc	0.775	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.89	J/mol×K	756.63	Joback Method
cpg	526.94	J/mol×K	798.09	Joback Method
cpg	538.82	J/mol×K	839.54	Joback Method
cpg	549.57	J/mol×K	881.00	Joback Method

cpg	559.25	J/mol×K	922.45	Joback Method
cpg	567.91	J/mol×K	963.91	Joback Method
cpg	575.60	J/mol×K	1005.36	Joback Method
dvisc	0.0009034	Paxs	453.69	Joback Method
dvisc	0.0005277	Paxs	504.18	Joback Method
dvisc	0.0003399	Paxs	554.67	Joback Method
dvisc	0.0002356	Paxs	605.16	Joback Method
dvisc	0.0001728	Paxs	655.65	Joback Method
dvisc	0.0001325	Paxs	706.14	Joback Method
dvisc	0.0001053	Paxs	756.63	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=C5359386&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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