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	m3/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	Pa×s	453.69	Joback Method
dvisc	0.0005277	Pa×s	504.18	Joback Method
dvisc	0.0003399	Pa×s	554.67	Joback Method
dvisc	0.0002356	Pa×s	605.16	Joback Method
dvisc	0.0001728	Pa×s	655.65	Joback Method
dvisc	0.0001325	Pa×s	706.14	Joback Method
dvisc	0.0001053	Pa×s	756.63	Joback Method

Sources

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
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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