

Diethylmalonic acid, monochloride, 2-formylphenyl ester

Inchi:	InChI=1S/C14H15ClO4/c1-3-14(4-2,12(15)17)13(18)19-11-8-6-5-7-10(11)9-16/h5-9H,3-4
InchiKey:	GDGUNMJGQMVI AZ-UHFFFAOYSA-N
Formula:	C14H15ClO4
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1ccccc1C=O
Mol. weight [g/mol]:	282.72

Physical Properties

Property code	Value	Unit	Source
gf	-301.67	kJ/mol	Joback Method
hf	-574.68	kJ/mol	Joback Method
hfus	29.13	kJ/mol	Joback Method
hvap	75.41	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.976		Crippen Method
mcvol	207.180	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinsol	1934.00		NIST Webbook
tb	764.40	K	Joback Method
tc	987.76	K	Joback Method
tf	482.91	K	Joback Method
vc	0.796	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.79	J/molxK	764.40	Joback Method
cpg	606.98	J/molxK	950.53	Joback Method
cpg	598.48	J/molxK	913.30	Joback Method
cpg	589.16	J/molxK	876.08	Joback Method
cpg	578.97	J/molxK	838.85	Joback Method
cpg	567.87	J/molxK	801.63	Joback Method
cpg	614.71	J/molxK	987.76	Joback Method
dvisc	0.0001257	Paxs	764.40	Joback Method
dvisc	0.0001601	Paxs	717.49	Joback Method

dvisc	0.0002110	Paxs	670.57	Joback Method
dvisc	0.0002899	Paxs	623.65	Joback Method
dvisc	0.0004193	Paxs	576.74	Joback Method
dvisc	0.0006474	Paxs	529.83	Joback Method
dvisc	0.0010878	Paxs	482.91	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=U369963&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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