

Diethylmalonic acid, monochloride, 4-fluoro-2-methoxyphenyl ester

Inchi:	InChI=1S/C14H16ClFO4/c1-4-14(5-2,12(15)17)13(18)20-10-7-6-9(16)8-11(10)19-3/h6-8
InchiKey:	XFBDUOPRRDUFD-UHFFFAOYSA-N
Formula:	C14H16ClFO4
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1ccc(F)cc1OC
Mol. weight [g/mol]:	302.73

Physical Properties

Property code	Value	Unit	Source
gf	-511.59	kJ/mol	Joback Method
hf	-828.90	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.311		Crippen Method
mcvol	213.250	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	742.41	K	Joback Method
tc	954.26	K	Joback Method
tf	476.25	K	Joback Method
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.06	J/mol×K	742.41	Joback Method
cpg	587.98	J/mol×K	777.72	Joback Method
cpg	599.97	J/mol×K	813.03	Joback Method
cpg	611.04	J/mol×K	848.33	Joback Method
cpg	621.23	J/mol×K	883.64	Joback Method
cpg	630.56	J/mol×K	918.95	Joback Method
cpg	639.05	J/mol×K	954.26	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=U370909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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