Diethylmalonic acid, monochloride, 2-methylthiophenyl ester

Inchi: InChI=1S/C14H17ClO3S/c1-4-14(5-2,12(15)16)13(17)18-10-8-6-7-9-11(10)19-3/h6-9H,4-

InchiKey: QOYLFIHGOKUTSU-UHFFFAOYSA-N

Formula: C14H17ClO3S

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1ccccc1SC

Mol. weight [g/mol]: 300.80

Physical Properties

Property code	Value	Unit	Source
gf	-169.03	kJ/mol	Joback Method
hf	-447.23	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	75.50	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.886		Crippen Method
mcvol	221.960	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	2045.00		NIST Webbook
tb	784.52	K	Joback Method
tc	1020.45	K	Joback Method
tf	475.31	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.38	J/mol×K	784.52	Joback Method
cpg	607.48	J/mol×K	823.84	Joback Method
cpg	619.45	J/mol×K	863.16	Joback Method
cpg	630.32	J/mol×K	902.48	Joback Method
cpg	640.15	J/mol×K	941.80	Joback Method
cpg	648.99	J/mol×K	981.12	Joback Method
cpg	656.90	J/mol×K	1020.45	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369544&Units=SI

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
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