Diethylmalonic acid, 2-methylthiophenyl propyl ester

Inchi: InChI=1S/C17H24O4S/c1-5-12-20-15(18)17(6-2,7-3)16(19)21-13-10-8-9-11-14(13)22-4/h

InchiKey: ANWMJFDTXABQTR-UHFFFAOYSA-N

Formula: C17H24O4S

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC

Mol. weight [g/mol]: 324.44

Physical Properties

Property code	Value	Unit	Source
gf	-236.84	kJ/mol	Joback Method
hf	-625.63	kJ/mol	Joback Method
hfus	35.73	kJ/mol	Joback Method
hvap	80.21	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.073		Crippen Method
mcvol	257.860	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	838.15	K	Joback Method
tc	1059.72	K	Joback Method
tf	501.43	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.18	J/mol×K	838.15	Joback Method
cpg	777.71	J/mol×K	875.08	Joback Method
cpg	791.01	J/mol×K	912.01	Joback Method
cpg	803.10	J/mol×K	948.93	Joback Method
cpg	814.03	J/mol×K	985.86	Joback Method
cpg	823.81	J/mol×K	1022.79	Joback Method
cpg	832.49	J/mol×K	1059.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369529&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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