Diethylmalonic acid, 2-methylthiophenyl pentyl ester

Inchi: InChI=1S/C19H28O4S/c1-5-8-11-14-22-17(20)19(6-2,7-3)18(21)23-15-12-9-10-13-16(15

InchiKey: XOIVTZFXAROWIQ-UHFFFAOYSA-N

Formula: C19H28O4S

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

Mol. weight [g/mol]: 352.49

Physical Properties

Property code	Value	Unit	Source
gf	-220.00	kJ/mol	Joback Method
hf	-666.91	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	84.66	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.854		Crippen Method
mcvol	286.040	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2365.00		NIST Webbook
tb	883.91	K	Joback Method
tc	1102.61	K	Joback Method
tf	523.97	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.56	J/mol×K	883.91	Joback Method
cpg	893.29	J/mol×K	920.36	Joback Method
cpg	906.75	J/mol×K	956.81	Joback Method
cpg	918.96	J/mol×K	993.26	Joback Method
cpg	929.97	J/mol×K	1029.71	Joback Method
cpg	939.82	J/mol×K	1066.16	Joback Method
cpg	948.54	J/mol×K	1102.61	Joback Method

Sources

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=U369532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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