Diethylmalonic acid, isobutyl 2-methylthiophenyl ester

Inchi: InChI=1S/C18H26O4S/c1-6-18(7-2,16(19)21-12-13(3)4)17(20)22-14-10-8-9-11-15(14)23

InchiKey: MOMQNSKGYNJAIK-UHFFFAOYSA-N

Formula: C18H26O4S

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

Mol. weight [g/mol]: 338.46

Physical Properties

Property code	Value	Unit	Source
gf	-230.86	kJ/mol	Joback Method
hf	-651.55	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	82.05	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.319		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	860.59	K	Joback Method
tc	1083.16	K	Joback Method
tf	497.70	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.03	J/mol×K	860.59	Joback Method
cpg	835.83	J/mol×K	897.69	Joback Method
cpg	849.33	J/mol×K	934.78	Joback Method
cpg	861.57	J/mol×K	971.88	Joback Method
cpg	872.59	J/mol×K	1008.97	Joback Method
cpg	882.41	J/mol×K	1046.07	Joback Method
cpg	891.07	J/mol×K	1083.16	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=U369530&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