Diethylmalonic acid, heptyl 2-methylthiophenyl ester

Inchi: InChI=1S/C21H32O4S/c1-5-8-9-10-13-16-24-19(22)21(6-2,7-3)20(23)25-17-14-11-12-15

InchiKey: MCJKHEAZUQZSKP-UHFFFAOYSA-N

Formula: C21H32O4S

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

Mol. weight [g/mol]: 380.54

Physical Properties

Property code	Value	Unit	Source
gf	-203.16	kJ/mol	Joback Method
hf	-708.19	kJ/mol	Joback Method
hfus	46.09	kJ/mol	Joback Method
hvap	89.11	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.634		Crippen Method
mcvol	314.220	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
rinpol	2556.00		NIST Webbook
tb	929.67	K	Joback Method
tc	1148.41	K	Joback Method
tf	546.51	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.76	J/mol×K	929.67	Joback Method
cpg	1011.64	J/mol×K	966.13	Joback Method
cpg	1025.18	J/mol×K	1002.58	Joback Method
cpg	1037.44	J/mol×K	1039.04	Joback Method
cpg	1048.44	J/mol×K	1075.49	Joback Method
cpg	1058.25	J/mol×K	1111.95	Joback Method
cpg	1066.90	J/mol×K	1148.41	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=U369534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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