Diethylmalonic acid, 2-methylthiophenyl octyl ester

Inchi: InChI=1S/C22H34O4S/c1-5-8-9-10-11-14-17-25-20(23)22(6-2,7-3)21(24)26-18-15-12-13

InchiKey: XQWFOAMWJNTPTN-UHFFFAOYSA-N

Formula: C22H34O4S

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

Mol. weight [g/mol]: 394.57

Physical Properties

Property code	Value	Unit	Source
gf	-194.74	kJ/mol	Joback Method
hf	-728.83	kJ/mol	Joback Method
hfus	48.68	kJ/mol	Joback Method
hvap	91.34	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.024		Crippen Method
mcvol	328.310	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
rinpol	2656.00		NIST Webbook
tb	952.55	K	Joback Method
tc	1172.52	K	Joback Method
tf	557.78	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.77	J/mol×K	952.55	Joback Method
cpg	1071.72	J/mol×K	989.21	Joback Method
cpg	1085.30	J/mol×K	1025.87	Joback Method
cpg	1097.56	J/mol×K	1062.53	Joback Method
cpg	1108.54	J/mol×K	1099.19	Joback Method
cpg	1118.30	J/mol×K	1135.86	Joback Method
cpg	1126.88	J/mol×K	1172.52	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=U369535&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