Glutaric acid, di(2-(methylthio)phenyl) ester

Inchi: InChI=1S/C19H20O4S2/c1-24-16-10-5-3-8-14(16)22-18(20)12-7-13-19(21)23-15-9-4-6-1
InchiKey: GDVGOLMFSKRRML-UHFFFAOYSA-N
Formula: C19H20O4S2
SMILES: CSc1ccccc1OC(=O)CCCC(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-86.94	kJ/mol	Joback Method
hf	-391.23	kJ/mol	Joback Method
hfus	46.10	kJ/mol	Joback Method
hvap	95.71	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.812		Crippen Method
mcvol	278.630	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	3315.00		NIST Webbook
rinpol	3315.00		NIST Webbook
tb	987.58	K	Joback Method
tc	1239.41	K	Joback Method
tf	594.89	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.57	J/mol×K	987.58	Joback Method
cpg	831.34	J/mol×K	1029.55	Joback Method
cpg	839.37	J/mol×K	1071.52	Joback Method
cpg	845.67	J/mol×K	1113.50	Joback Method
cpg	850.25	J/mol×K	1155.47	Joback Method
cpg	853.13	J/mol×K	1197.44	Joback Method
cpg	854.32	J/mol×K	1239.41	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=U377544&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