Glutaric acid, ethyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C14H18O4S/c1-3-17-13(15)9-6-10-14(16)18-11-7-4-5-8-12(11)19-2/h4-5,7-8H
InchiKey: ACKAYLPYEPAPTE-UHFFFAOYSA-N
Formula: C14H18O4S
SMILES: CCOC(=O)CCCC(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 282.36

Physical Properties

Property code	Value	Unit	Source
gf	-264.94	kJ/mol	Joback Method
hf	-554.96	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	74.83	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.047		Crippen Method
mcvol	215.590	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	2316.00		NIST Webbook
tb	772.74	K	Joback Method
tc	992.64	K	Joback Method
tf	465.20	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.43	J/mol×K	772.74	Joback Method
cpg	608.07	J/mol×K	809.39	Joback Method
cpg	620.63	J/mol×K	846.04	Joback Method
cpg	632.12	J/mol×K	882.69	Joback Method
cpg	642.54	J/mol×K	919.34	Joback Method
cpg	651.87	J/mol×K	955.99	Joback Method
cpg	660.13	J/mol×K	992.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377536&Units=SI
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

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