Glutaric acid, heptyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C19H28O4S/c1-3-4-5-6-9-15-22-18(20)13-10-14-19(21)23-16-11-7-8-12-17(16

InchiKey: XJJCTJMBWBQBQC-UHFFFAOYSA-N

Formula: C19H28O4S

SMILES: CCCCCCCOC(=O)CCCC(=O)Oc1ccccc1SC

Mol. weight [g/mol]: 352.49

Physical Properties

Property code	Value	Unit	Source
gf	-222.84	kJ/mol	Joback Method
hf	-658.16	kJ/mol	Joback Method
hfus	48.32	kJ/mol	Joback Method
hvap	85.95	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.998		Crippen Method
mcvol	286.040	ml/mol	McGowan Method
pc	1460.13	kPa	Joback Method
rinpol	2884.00		NIST Webbook
tb	887.14	K	Joback Method
tc	1099.93	K	Joback Method
tf	521.55	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.76	J/mol×K	887.14	Joback Method
cpg	892.30	J/mol×K	922.60	Joback Method
cpg	905.56	J/mol×K	958.07	Joback Method
cpg	917.57	J/mol×K	993.53	Joback Method
cpg	928.32	J/mol×K	1029.00	Joback Method
cpg	937.85	J/mol×K	1064.46	Joback Method
cpg	946.16	J/mol×K	1099.93	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=U377543&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