Glutaric acid, 2-methylhex-3-yl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C19H28O4S/c1-5-9-15(14(2)3)22-18(20)12-8-13-19(21)23-16-10-6-7-11-17(16

InchiKey: NXKKMLRRXUFKKZ-UHFFFAOYSA-N

Formula: C19H28O4S

SMILES: CCCC(OC(=O)CCCC(=O)Oc1ccccc1SC)C(C)C

Mol. weight [g/mol]: 352.49

Physical Properties

Property code	Value	Unit	Source
gf	-227.72	kJ/mol	Joback Method
hf	-668.72	kJ/mol	Joback Method
hfus	41.28	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.852		Crippen Method
mcvol	286.040	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2717.00		NIST Webbook
tb	886.26	K	Joback Method
tc	1103.17	K	Joback Method
tf	491.55	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.79	J/mol×K	886.26	Joback Method
cpg	893.55	J/mol×K	922.41	Joback Method
cpg	906.96	J/mol×K	958.56	Joback Method
cpg	919.04	J/mol×K	994.72	Joback Method
cpg	929.80	J/mol×K	1030.87	Joback Method
cpg	939.26	J/mol×K	1067.02	Joback Method
cpg	947.43	J/mol×K	1103.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377541&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