Glutaric acid, hexyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C18H26O4S/c1-3-4-5-8-14-21-17(19)12-9-13-18(20)22-15-10-6-7-11-16(15)23
InchiKey: YTEWGVMEUBJFQR-UHFFFAOYSA-N
Formula: C18H26O4S
SMILES: CCCCCCOC(=O)CCCC(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 338.46

Physical Properties

Property code	Value	Unit	Source
gf	-231.26	kJ/mol	Joback Method
hf	-637.52	kJ/mol	Joback Method
hfus	45.73	kJ/mol	Joback Method
hvap	83.73	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.608		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1573.45	kPa	Joback Method
rinpol	2775.00		NIST Webbook
tb	864.26	K	Joback Method
tc	1077.15	K	Joback Method
tf	510.28	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.46	J/mol×K	864.26	Joback Method
cpg	833.88	J/mol×K	899.74	Joback Method
cpg	847.08	J/mol×K	935.22	Joback Method
cpg	859.05	J/mol×K	970.70	Joback Method
cpg	869.82	J/mol×K	1006.19	Joback Method
cpg	879.39	J/mol×K	1041.67	Joback Method
cpg	887.79	J/mol×K	1077.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377542&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