Glutaric acid, 2-(methylthio)phenyl propyl ester

Inchi: InChI=1S/C15H20O4S/c1-3-11-18-14(16)9-6-10-15(17)19-12-7-4-5-8-13(12)20-2/h4-5,7-

InchiKey: OORWFXCQLAZLNX-UHFFFAOYSA-N

Formula: C15H20O4S

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

Mol. weight [g/mol]: 296.38

Physical Properties

Property code	Value	Unit	Source
gf	-256.52	kJ/mol	Joback Method
hf	-575.60	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	77.05	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.437		Crippen Method
mcvol	229.680	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	2434.00		NIST Webbook
tb	795.62	K	Joback Method
tc	1012.87	K	Joback Method
tf	476.47	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.30	J/mol×K	795.62	Joback Method
cpg	663.21	J/mol×K	831.83	Joback Method
cpg	676.01	J/mol×K	868.04	Joback Method
cpg	687.69	J/mol×K	904.24	Joback Method
cpg	698.26	J/mol×K	940.45	Joback Method
cpg	707.73	J/mol×K	976.66	Joback Method
cpg	716.10	J/mol×K	1012.87	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=U377537&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