Glutaric acid, isobutyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C16H22O4S/c1-12(2)11-19-15(17)9-6-10-16(18)20-13-7-4-5-8-14(13)21-3/h4-5

InchiKey: RHFYPLIBUPAFFV-UHFFFAOYSA-N

Formula: C16H22O4S

SMILES: CSc1ccccc1OC(=O)CCCC(=O)OCC(C)C

Mol. weight [g/mol]: 310.41

Physical Properties

Property code	Value	Unit	Source
gf	-250.54	kJ/mol	Joback Method
hf	-601.52	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.683		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2494.00		NIST Webbook
tb	818.06	K	Joback Method
tc	1036.20	K	Joback Method
tf	472.74	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.72	J/mol×K	818.06	Joback Method
cpg	720.02	J/mol×K	854.42	Joback Method
cpg	733.13	J/mol×K	890.77	Joback Method
cpg	745.05	J/mol×K	927.13	Joback Method
cpg	755.79	J/mol×K	963.49	Joback Method
cpg	765.34	J/mol×K	999.84	Joback Method
cpg	773.74	J/mol×K	1036.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377538&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

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