2-(Methylthio)benzoic acid anhydride

Inchi: InChI=1S/C16H14O3S2/c1-20-13-9-5-3-7-11(13)15(17)19-16(18)12-8-4-6-10-14(12)21-2
InchiKey: XMXDDBIWASGZCG-UHFFFAOYSA-N
Formula: C16H14O3S2
SMILES: CSc1ccccc1C(=O)OC(=O)c1ccccc1SC
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-7.20	kJ/mol	Joback Method
hf	-197.09	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	86.62	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.128		Crippen Method
mcvol	230.490	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	2818.00		NIST Webbook
tb	896.52	K	Joback Method
tc	1163.37	K	Joback Method
tf	538.85	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.38	J/mol×K	896.52	Joback Method
cpg	639.30	J/mol×K	940.99	Joback Method
cpg	648.65	J/mol×K	985.47	Joback Method
cpg	656.45	J/mol×K	1029.94	Joback Method
cpg	662.73	J/mol×K	1074.42	Joback Method
cpg	667.52	J/mol×K	1118.89	Joback Method
cpg	670.84	J/mol×K	1163.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374994&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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