

Benzoic acid, thio-2,2'-di

Inchi:	InChI=1S/C14H10O4S/c15-13(16)9-5-1-3-7-11(9)19-12-8-4-2-6-10(12)14(17)18/h1-8H,(H
InchiKey:	BDUPKZTWQYDOGC-UHFFFAOYSA-N
Formula:	C14H10O4S
SMILES:	O=C(O)c1ccccc1Sc1ccccc1C(=O)O
Mol. weight [g/mol]:	274.29
CAS:	22219-02-9

Physical Properties

Property code	Value	Unit	Source
gf	-225.80	kJ/mol	Joback Method
hf	-369.92	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	106.30	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.234		Crippen Method
mcvol	191.830	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	943.92	K	Joback Method
tc	1177.65	K	Joback Method
tf	581.32	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.84	J/molxK	943.92	Joback Method
cpg	537.69	J/molxK	982.87	Joback Method
cpg	543.73	J/molxK	1021.83	Joback Method
cpg	549.02	J/molxK	1060.78	Joback Method
cpg	553.60	J/molxK	1099.74	Joback Method
cpg	557.51	J/molxK	1138.69	Joback Method
cpg	560.81	J/molxK	1177.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22219029&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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