

3,6-Diphenyl-1,2-dithiin

Inchi:	InChI=1S/C16H12S2/c1-3-7-13(8-4-1)15-11-12-16(18-17-15)14-9-5-2-6-10-14/h1-12H
InchiKey:	TWFJKRAZUIJOSQ-UHFFFAOYSA-N
Formula:	C16H12S2
SMILES:	C1=C(c2ccccc2)SSC(c2ccccc2)=C1
Mol. weight [g/mol]:	268.40
CAS:	16212-85-4

Physical Properties

Property code	Value	Unit	Source
chs	-9455.00	kJ/mol	NIST Webbook
gf	461.20	kJ/mol	Joback Method
hf	422.40 ± 3.60	kJ/mol	NIST Webbook
hfus	25.02	kJ/mol	Joback Method
hsub	183.10 ± 2.50	kJ/mol	NIST Webbook
hsub	183.10 ± 2.50	kJ/mol	NIST Webbook
hvap	70.03	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.464		Crippen Method
mcvol	202.020	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	747.00	K	Joback Method
tc	1048.55	K	Joback Method
tf	528.00	K	Joback Method
vc	0.714	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.79	J/mol×K	998.29	Joback Method
cpg	503.76	J/mol×K	747.00	Joback Method
cpg	520.02	J/mol×K	797.26	Joback Method
cpg	534.57	J/mol×K	847.52	Joback Method
cpg	547.59	J/mol×K	897.77	Joback Method
cpg	559.27	J/mol×K	948.03	Joback Method

cpg	579.34	J/mol×K	1048.55	Joback Method
hsubt	174.50 ± 2.50	kJ/mol	355.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16212854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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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