Thiirane,trans-2,3-diethynyl-

Inchi: InChI=1S/C6H4S/c1-3-5-6(4-2)7-5/h1-2,5-6H/t5-,6-/m0/s1
InchiKey: ZEODDVBXGCQFTC-WDSKDSINSA-N
Formula: C6H4S
SMILES: C#CC1SC1C#C
Mol. weight [g/mol]: 108.16
CAS: 50555-55-0

Physical Properties

Property code	Value	Unit	Source
gf	538.68	kJ/mol	Joback Method
hf	514.35	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	34.08	kJ/mol	Joback Method
ie	8.85	eV	NIST Webbook
log10ws	-1.93		Crippen Method
logp	0.737		Crippen Method
mcvol	83.690	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
tb	366.82	K	Joback Method
tc	594.35	K	Joback Method
tf	348.47	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.44	J/mol×K	366.82	Joback Method
cpg	148.35	J/mol×K	404.74	Joback Method
cpg	156.51	J/mol×K	442.66	Joback Method
cpg	163.97	J/mol×K	480.59	Joback Method
cpg	170.79	J/mol×K	518.51	Joback Method
cpg	177.02	J/mol×K	556.43	Joback Method
cpg	182.73	J/mol×K	594.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50555550&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
ie:	Ionization energy
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