Thiirane, 2,3-bis(1,1-tert-butyl)-, trans-

Inchi: InChI=1S/C10H20S/c1-9(2,3)7-8(11-7)10(4,5)6/h7-8H,1-6H3
InchiKey: SUKBJBHRMICECN-UHFFFAOYSA-N
Formula: C10H20S
SMILES: CC(C)(C)C1SC1C(C)(C)C
Mol. weight [g/mol]: 172.33
CAS: 52908-35-7

Physical Properties

Property code	Value	Unit	Source
gf	131.90	kJ/mol	Joback Method
hf	-169.51	kJ/mol	Joback Method
hfus	9.69	kJ/mol	Joback Method
hvap	40.68	kJ/mol	Joback Method
ie	8.39 ± 0.05	eV	NIST Webbook
log10ws	-3.53		Crippen Method
logp	3.563		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
tb	471.64	K	Joback Method
tc	685.03	K	Joback Method
tf	304.45	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.22	J/mol×K	471.64	Joback Method
cpg	378.05	J/mol×K	507.20	Joback Method
cpg	396.50	J/mol×K	542.77	Joback Method
cpg	413.67	J/mol×K	578.33	Joback Method
cpg	429.65	J/mol×K	613.90	Joback Method
cpg	444.52	J/mol×K	649.46	Joback Method
cpg	458.38	J/mol×K	685.03	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52908357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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