2-Tert-butyl,cis-4,cis-6-dimethyl-1,3-dithiane

Inchi: InChI=1S/C10H20S2/c1-7-6-8(2)12-9(11-7)10(3,4)5/h7-9H,6H2,1-5H3
InchiKey: MFVZIKOLBGYKSR-UHFFFAOYSA-N
Formula: C10H20S2
SMILES: CC1CC(C)SC(C(C)(C)C)S1
Mol. weight [g/mol]: 204.40
CAS: 22425-92-9

Physical Properties

Property code	Value	Unit	Source
gf	124.91	kJ/mol	Joback Method
hf	-154.32	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	47.99	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.006		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	530.84	K	Joback Method
tc	768.38	K	Joback Method
tf	370.68	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.74	J/mol×K	530.84	Joback Method
cpg	431.28	J/mol×K	570.43	Joback Method
cpg	451.44	J/mol×K	610.02	Joback Method
cpg	470.27	J/mol×K	649.61	Joback Method
cpg	487.82	J/mol×K	689.20	Joback Method
cpg	504.15	J/mol×K	728.79	Joback Method
cpg	519.33	J/mol×K	768.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22425929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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