trans, cis-2-Methyl-1-thiadecalin

Inchi: InChI=1S/C12H22S/c1-10-6-9-11(2)7-4-5-8-12(11,3)13-10/h10H,4-9H2,1-3H3/t10-,11+,1
InchiKey: YSNQSSXOPDJTBK-GRYCIOLGSA-N
Formula: C10H18S
SMILES: CC1CCC2(C)CCCCC2(C)S1
Mol. weight [g/mol]: 170.31
CAS: 42900-29-8

Physical Properties

Property code	Value	Unit	Source
gf	144.43	kJ/mol	Joback Method
hf	-114.65	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	46.02	kJ/mol	Joback Method
ie	7.86 ± 0.01	eV	NIST Webbook
log10ws	-4.50		Crippen Method
logp	4.241		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	548.16	K	Joback Method
tc	795.75	K	Joback Method
tf	373.81	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.64	J/mol×K	548.16	Joback Method
cpg	462.07	J/mol×K	589.43	Joback Method
cpg	483.74	J/mol×K	630.69	Joback Method
cpg	503.96	J/mol×K	671.96	Joback Method
cpg	523.08	J/mol×K	713.22	Joback Method
cpg	541.42	J/mol×K	754.49	Joback Method
cpg	559.31	J/mol×K	795.75	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=C42900298&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