2-Thiiranebutanenitrile

Inchi: InChI=1S/C6H9NS/c7-4-2-1-3-6-5-8-6/h6H,1-3,5H2
InchiKey: GWYOVZVXBRVBBE-UHFFFAOYSA-N
Formula: C6H9NS
SMILES: N#CCCCC1CS1
Mol. weight [g/mol]: 127.21
CAS: 58130-94-2

Physical Properties

Property code	Value	Unit	Source
gf	233.43	kJ/mol	Joback Method
hf	115.77	kJ/mol	Joback Method
hfus	14.59	kJ/mol	Joback Method
hvap	45.15	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.796		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	1249.50		NIST Webbook
rinpol	1249.50		NIST Webbook
tb	493.33	K	Joback Method
tc	712.05	K	Joback Method
tf	323.76	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.68	J/mol×K	493.33	Joback Method
cpg	223.85	J/mol×K	529.78	Joback Method
cpg	233.34	J/mol×K	566.24	Joback Method
cpg	242.20	J/mol×K	602.69	Joback Method
cpg	250.49	J/mol×K	639.14	Joback Method
cpg	258.25	J/mol×K	675.60	Joback Method
cpg	265.52	J/mol×K	712.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58130942&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume