Pentane, 2-isothiocyanato-2,4,4-trimethyl-

Other names:	tert-Octyl isothiocyanate
	1,1,3,3-tetramethylbutyl isothiocyanate
Inchi:	InChI=1S/C9H17NS/c1-8(2,3)6-9(4,5)10-7-11/h6H2,1-5H3
InchiKey:	KUGHMFIBHMZICO-UHFFFAOYSA-N
Formula:	C9H17NS
SMILES:	CC(C)(C)CC(C)(C)N=C=S
Mol. weight [g/mol]:	171.30
CAS:	17701-76-7

Physical Properties

Property code	Value	Unit	Source
hf	37.48	kJ/mol	Joback Method
hvap	43.48	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.304		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
tb	544.81	K	Joback Method
tc	776.74	K	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=C17701767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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