

tert-Nonyl mercaptan

Other names:	tert-Nonanethiol 1,1-dimethylheptanethiol
Inchi:	InChI=1S/C9H20S/c1-4-5-6-7-8-9(2,3)10/h10H,4-8H2,1-3H3
InchiKey:	MPBLPZLNKKGCGP-UHFFFAOYSA-N
Formula:	C9H20S
SMILES:	CCCCCCC(C)(C)S
Mol. weight [g/mol]:	160.32
CAS:	25360-10-5

Physical Properties

Property code	Value	Unit	Source
gf	57.13	kJ/mol	Joback Method
hf	-199.36	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	41.07	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.665		Crippen Method
mvol	154.020	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	464.95	K	Joback Method
tc	660.46	K	Joback Method
tf	230.07	K	Joback Method
vc	0.583	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.39	J/molxK	464.95	Joback Method
cpg	346.59	J/molxK	497.54	Joback Method
cpg	361.94	J/molxK	530.12	Joback Method
cpg	376.48	J/molxK	562.71	Joback Method
cpg	390.23	J/molxK	595.29	Joback Method
cpg	403.24	J/molxK	627.88	Joback Method
cpg	415.54	J/molxK	660.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25360105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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

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