

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]:	160.33

Physical Properties

Property code	Value	Unit	Source
af	0.4772		Cheméo Relay (1.0)
gf	57.13	kJ/mol	Joback Method
hf	-213.44	kJ/mol	Cheméo Relay (1.0)
hfus	15.69	kJ/mol	Joback Method
hvap	51.55	kJ/mol	Cheméo Relay (1.0)
ie	8.87	eV	Cheméo Relay (1.0)
log10ws	-4.51		Cheméo Relay (1.0)
logp	3.665		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	449.79	K	Cheméo Relay (1.0)
tc	642.70	K	Cheméo Relay (1.0)
tf	232.76	K	Cheméo Relay (1.0)
vc	0.566	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25360105&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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

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