Tert-dodecyl mercaptan

Other names: Decanethiol, 9,9-dimethyl-
Inchi: InChI=1S/C12H26S/c1-12(2,3)10-8-6-4-5-7-9-11-13/h13H,4-11H2,1-3H3
InchiKey: UVXGZLRXSOTRRS-UHFFFAOYSA-N
Formula: C12H26S
SMILES: CC(C)(C)CCCCCCCCS
Mol. weight [g/mol]: 202.40
CAS: 7341-22-2

Physical Properties

Property code	Value	Unit	Source
gf	82.39	kJ/mol	Joback Method
hf	-261.28	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	47.75	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.693		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
tb	533.59	K	Joback Method
tc	722.19	K	Joback Method
tf	263.88	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.83	J/mol×K	533.59	Joback Method
cpg	490.12	J/mol×K	565.02	Joback Method
cpg	507.49	J/mol×K	596.46	Joback Method
cpg	523.96	J/mol×K	627.89	Joback Method
cpg	539.59	J/mol×K	659.32	Joback Method
cpg	554.41	J/mol×K	690.75	Joback Method
cpg	568.46	J/mol×K	722.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7341222&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume