7-Thia-1-octanethiol

Inchi: InChI=1S/C7H16S2/c1-9-7-5-3-2-4-6-8/h8H,2-7H2,1H3
InchiKey: MCCWTNNEODFSQN-UHFFFAOYSA-N
Formula: C7H16S2
SMILES: CSCCCCCCS
Mol. weight [g/mol]: 164.33

Physical Properties

Property code	Value	Unit	Source
gf	70.57	kJ/mol	Joback Method
hf	-107.46	kJ/mol	Joback Method
hfus	22.06	kJ/mol	Joback Method
hvap	44.73	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.840		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
tb	491.20	K	Joback Method
tc	700.51	K	Joback Method
tf	239.51	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.29	J/mol×K	491.20	Joback Method
cpg	307.70	J/mol×K	526.08	Joback Method
cpg	320.47	J/mol×K	560.97	Joback Method
cpg	332.63	J/mol×K	595.85	Joback Method
cpg	344.17	J/mol×K	630.74	Joback Method
cpg	355.13	J/mol×K	665.62	Joback Method
cpg	365.50	J/mol×K	700.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157672&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

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

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