

3-heptanethiol

Inchi:	InChI=1S/C7H16S/c1-3-5-6-7(8)4-2/h7-8H,3-6H2,1-2H3
InchiKey:	CTLFTVHSIFCSNE-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CCCCC(S)CC
Mol. weight [g/mol]:	132.27
CAS:	---

Physical Properties

Property code	Value	Unit	Source
gf	35.01	kJ/mol	Joback Method
hf	-154.61	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	37.52	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.885		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
ripol	1157.60		NIST Webbook
ripol	1153.20		NIST Webbook
ripol	1157.60		NIST Webbook
tb	421.98	K	Joback Method
tc	613.54	K	Joback Method
tf	190.11	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.65	J/mol×K	421.98	Joback Method
cpg	256.79	J/mol×K	453.91	Joback Method
cpg	269.35	J/mol×K	485.83	Joback Method
cpg	281.37	J/mol×K	517.76	Joback Method
cpg	292.85	J/mol×K	549.69	Joback Method
cpg	303.81	J/mol×K	581.61	Joback Method

cpg

314.27

J/mol×K

613.54

Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43263e+01
Coeff. B	-3.73865e+03
Coeff. C	-6.22880e+01
Temperature range (K), min.	328.60
Temperature range (K), max.	477.01

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R295848&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:

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
pvap:	Vapor pressure
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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