3-Pentanethiol

Other names:	pentane-3-thiol
Inchi:	InChI=1S/C5H12S/c1-3-5(6)4-2/h5-6H,3-4H2,1-2H3
InchiKey:	WICKAMSPKJXSGN-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCC(S)CC
Mol. weight [g/mol]:	104.21
CAS:	616-31-9

Physical Properties

Property code	Value	Unit	Source
gf	18.17	kJ/mol	Joback Method
hf	-113.33	kJ/mol	Joback Method
hfus	9.22	kJ/mol	Joback Method
hvap	33.07	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.105		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	758.00		NIST Webbook
rinpol	758.00		NIST Webbook
ripol	973.90		NIST Webbook
ripol	979.50		NIST Webbook
tb	387.05 ± 0.20	K	NIST Webbook
tc	570.72	K	Joback Method
tf	167.57	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.28	J/mol×K	376.22	Joback Method
cpg	178.71	J/mol×K	408.64	Joback Method
cpg	188.71	J/mol×K	441.05	Joback Method
cpg	198.28	J/mol×K	473.47	Joback Method

cpg	207.43	J/mol×K	505.89	Joback Method
cpg	216.18	J/mol×K	538.31	Joback Method
cpg	224.53	J/mol×K	570.72	Joback Method
hvapt	38.30	kJ/mol	350.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53900e+01
Coeff. B	-3.64407e+03
Coeff. C	-4.87500e+01
Temperature range (K), min.	290.04
Temperature range (K), max.	410.32

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616319&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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