2-Pentanethiol

Other names:	1-Methylbutanethiol
	2-Mercaptopentane
	2-Pentylthiol
	Pentane-2-thiol
	sec-Amyl mercaptan
Inchi:	InChI=1S/C5H12S/c1-3-4-5(2)6/h5-6H,3-4H2,1-2H3
InchiKey:	QUSTYFNPKBDELJ-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCCC(C)S
Mol. weight [g/mol]:	104.21
CAS:	2084-19-7

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	782.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	751.00		NIST Webbook
ripol	967.90		NIST Webbook
ripol	992.00		NIST Webbook
ripol	964.90		NIST Webbook
tb	376.22	K	Joback Method
tc	570.72	K	Joback Method
tf	104.20 ± 0.30	K	NIST Webbook
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	38.40	kJ/mol	349.50	NIST Webbook
hvapt	37.80	kJ/mol	391.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41096e+01
Coeff. B	-3.32428e+03
Coeff. C	-4.83330e+01
Temperature range (K), min.	288.84
Temperature range (K), max.	426.17

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1828

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2084197&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

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