2-Octanethiol

Other names: 2-Octylthiol
octane-2-thiol
Inchi: InChI=1S/C8H18S/c1-3-4-5-6-7-8(2)9/h8-9H,3-7H2,1-2H3
InchiKey: BZXFEMZFRLXGCY-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CCCCCCC(C)S
Mol. weight [g/mol]: 146.29
CAS: 3001-66-9

Physical Properties

Property code	Value	Unit	Source
gf	43.43	kJ/mol	Joback Method
hf	-175.25	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	39.75	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.275		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
ripol	1298.00		NIST Webbook
tb	444.86	K	Joback Method
tc	634.61	K	Joback Method
tf	194.20 ± 0.30	K	NIST Webbook
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.76	J/mol×K	444.86	Joback Method
cpg	299.03	J/mol×K	476.48	Joback Method
cpg	312.67	J/mol×K	508.11	Joback Method

cpg	325.72	J/mol×K	539.73	Joback Method
cpg	338.18	J/mol×K	571.36	Joback Method
cpg	350.07	J/mol×K	602.98	Joback Method
cpg	361.41	J/mol×K	634.61	Joback Method
hvapt	49.00	kJ/mol	418.00	NIST Webbook

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=C3001669&Units=SI
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
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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