2-heptanethiol

Inchi: InChI=1S/C7H16S/c1-3-4-5-6-7(2)8/h7-8H,3-6H2,1-2H3
InchiKey: DAZNOIJJVKASGS-UHFFFAOYSA-N
Formula: C7H16S
SMILES: CCCCCC(C)S
Mol. weight [g/mol]: 132.27
CAS: 1628-00-2

Physical Properties

Property code	Value	Unit	Source
af	0.4219		Cheméo Relay (1.0)
gf	35.01	kJ/mol	Joback Method
hf	-171.26	kJ/mol	Cheméo Relay (1.0)
hfus	14.40	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-3.53		Cheméo Relay (1.0)
logp	2.885		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	426.56	K	Cheméo Relay (1.0)
tc	617.11	K	Cheméo Relay (1.0)
tf	165.88	K	Cheméo Relay (1.0)
vc	0.468	m3/kmol	Cheméo Relay (1.0)

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(Pvp) = A + B/(T + C)
Coeff. A	1.44593e+01
Coeff. B	-3.78714e+03
Coeff. C	-6.25660e+01
Temperature range (K), min.	329.80
Temperature range (K), max.	476.56

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628002&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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