2-Heptylthiol

Other names: 2-heptanethiol
heptane-2-thiol
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: 628-00-2

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
rinpol	983.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1165.50		NIST Webbook
tb	437.00 ± 3.00	K	NIST Webbook
tc	613.54	K	Joback Method
tf	132.20 ± 0.30	K	NIST Webbook
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
hvapt	44.10	kJ/mol	390.00	NIST Webbook
hvapt	47.20	kJ/mol	407.00	NIST Webbook
hvapt	44.20	kJ/mol	392.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628002&Units=SI

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