1-HEXANOL, 6-MERCAPTO-

Other names: 6-Mercaptohexanol
Inchi: InChI=1S/C6H14OS/c7-5-3-1-2-4-6-8/h7-8H,1-6H2
InchiKey: UGZAJZLUKVKCBM-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: OCCCCCCS
Mol. weight [g/mol]: 134.24

Physical Properties

Property code	Value	Unit	Source
af	0.7001		Cheméo Relay (1.0)
gf	-107.79	kJ/mol	Joback Method
hf	-286.48	kJ/mol	Cheméo Relay (1.0)
hfus	19.43	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Cheméo Relay (1.0)
ie	9.21	eV	Cheméo Relay (1.0)
log10ws	-1.39		Cheméo Relay (1.0)
logp	1.469		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2084.00		NIST Webbook
tb	509.84	K	Cheméo Relay (1.0)
tc	741.93	K	Cheméo Relay (1.0)
tf	279.66	K	Cheméo Relay (1.0)
vc	0.424	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.96	J/mol×K	491.72	Joback Method
cpg	262.98	J/mol×K	521.79	Joback Method

cpg	272.57	J/mol×K	551.85	Joback Method
cpg	281.74	J/mol×K	581.92	Joback Method
cpg	290.51	J/mol×K	611.98	Joback Method
cpg	298.89	J/mol×K	642.05	Joback Method
cpg	306.88	J/mol×K	672.12	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1633789&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

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

Cheméo Relay (1.0):

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
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