

1-PROPANOL, 3,3'-THIOBIS-

Other names:	1-Propanol, 3,3'-thiobis- Thiodipropanol 3,3'-thiodipropan-1-ol
Inchi:	InChI=1S/C6H14O2S/c7-3-1-5-9-6-2-4-8/h7-8H,1-6H2
InchiKey:	QRQVZZMTKYXEKC-UHFFFAOYSA-N
Formula:	C6H14O2S
SMILES:	OCCCCSCCO
Mol. weight [g/mol]:	150.24

Physical Properties

Property code	Value	Unit	Source
hf	-419.49	kJ/mol	Cheméo Relay (1.0)
hfus	23.60	kJ/mol	Joback Method
hvap	103.32	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
logp	0.484		Crippen Method
mcvol	123.490	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	574.71	K	Cheméo Relay (1.0)
tc	808.60	K	Cheméo Relay (1.0)
tf	288.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.13	J/mol×K	589.82	Joback Method
cpg	309.86	J/mol×K	618.67	Joback Method
cpg	318.22	J/mol×K	647.51	Joback Method
cpg	326.21	J/mol×K	676.36	Joback Method
cpg	333.84	J/mol×K	705.21	Joback Method
cpg	341.11	J/mol×K	734.06	Joback Method
cpg	348.04	J/mol×K	762.90	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10595092&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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