

Thiodipropylamine

Inchi:	InChI=1S/C6H16N2S/c7-3-1-5-9-6-2-4-8/h1-8H2
InchiKey:	QPIOXOJERGNNMX-UHFFFAOYSA-N
Formula:	C6H16N2S
SMILES:	NCCCSCCCN
Mol. weight [g/mol]:	148.27
CAS:	13643-20-4

Physical Properties

Property code	Value	Unit	Source
gf	165.66	kJ/mol	Joback Method
hf	-57.72	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.417		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
tb	550.52	K	Joback Method
tc	762.95	K	Joback Method
tf	358.30	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.25	J/mol×K	550.52	Joback Method
cpg	326.57	J/mol×K	585.92	Joback Method
cpg	338.26	J/mol×K	621.33	Joback Method
cpg	349.32	J/mol×K	656.73	Joback Method
cpg	359.79	J/mol×K	692.14	Joback Method
cpg	369.66	J/mol×K	727.54	Joback Method
cpg	378.95	J/mol×K	762.95	Joback Method

Sources

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=C13643204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
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
vc:	Critical Volume

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