

2,4,4-trimethylpentane-2-thiol

Inchi:	InChI=1S/C8H18S/c1-7(2,3)6-8(4,5)9/h9H,6H2,1-5H3
InchiKey:	QZLAEIZEPJAELS-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CC(C)(C)CC(C)(C)S
Mol. weight [g/mol]:	146.30

Physical Properties

Property code	Value	Unit	Source
gf	51.55	kJ/mol	Joback Method
hf	-187.47	kJ/mol	Joback Method
hfus	5.69	kJ/mol	Joback Method
hvap	37.55	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.131		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	438.84	K	Joback Method
tc	650.15	K	Joback Method
tf	221.22	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.20	J/molxK	438.84	Joback Method
cpg	306.07	J/molxK	474.06	Joback Method
cpg	321.84	J/molxK	509.28	Joback Method
cpg	336.56	J/molxK	544.50	Joback Method
cpg	350.30	J/molxK	579.72	Joback Method
cpg	363.12	J/molxK	614.93	Joback Method
cpg	375.08	J/molxK	650.15	Joback Method

Sources

KDB:	https://www.chemic.org/files/research/kdb/mol/mol1842.mol
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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