

trans-4-Methylcyclohexane-1-thiol

Inchi: InChI=1S/C7H14S/c1-6-2-4-7(8)5-3-6/h6-8H,2-5H2,1H3/t6-,7-
InchiKey: JYGRMXYSBUHFOS-LJGSYFOKSA-N
Formula: C7H14S
SMILES: CC1CCC(S)CC1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	54.19	kJ/mol	Joback Method
hf	-115.35	kJ/mol	Joback Method
hfus	10.83	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.495		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	985.00		NIST Webbook
tb	437.30	K	Joback Method
tc	666.53	K	Joback Method
tf	208.25	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.46	J/mol×K	437.30	Joback Method
cpg	243.00	J/mol×K	475.50	Joback Method
cpg	259.60	J/mol×K	513.71	Joback Method
cpg	275.28	J/mol×K	551.91	Joback Method
cpg	290.07	J/mol×K	590.12	Joback Method
cpg	303.98	J/mol×K	628.32	Joback Method
cpg	317.03	J/mol×K	666.53	Joback Method

Sources

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=R524319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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