2-(1-methylbutyl)thiazolidine

Inchi: InChI=1S/C8H17NS/c1-3-4-7(2)8-9-5-6-10-8/h7-9H,3-6H2,1-2H3
InchiKey: KEJJWLNKKYPOIN-UHFFFAOYSA-N
Formula: C8H17NS
SMILES: CCCC(C)C1NCCS1
Mol. weight [g/mol]: 159.29
CAS: 40790-75-8

Physical Properties

Property code	Value	Unit	Source
gf	178.16	kJ/mol	Joback Method
hf	-70.18	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.085		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	1254.00		NIST Webbook
tb	493.66	K	Joback Method
tc	713.18	K	Joback Method
tf	364.30	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.72	J/mol×K	493.66	Joback Method
cpg	324.85	J/mol×K	530.25	Joback Method
cpg	341.06	J/mol×K	566.83	Joback Method
cpg	356.38	J/mol×K	603.42	Joback Method
cpg	370.85	J/mol×K	640.01	Joback Method
cpg	384.48	J/mol×K	676.59	Joback Method
cpg	397.31	J/mol×K	713.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40790758&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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