2-isobutyl-4-methyl-3-thiazoline

Inchi: InChI=1S/C8H15NS/c1-6(2)4-8-9-7(3)5-10-8/h6,8H,4-5H2,1-3H3
InchiKey: WGLZXNQVSYIJRY-UHFFFAOYSA-N
Formula: C8H15NS
SMILES: CC1=NC(CC(C)C)SC1
Mol. weight [g/mol]: 157.28

Physical Properties

Property code	Value	Unit	Source
gf	227.56	kJ/mol	Joback Method
hf	9.29	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	46.25	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.566		Crippen Method
mcvol	134.750	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1228.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1228.00		NIST Webbook
ripol	1630.00		NIST Webbook
tb	502.95	K	Joback Method
tc	730.35	K	Joback Method
tf	344.09	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.40	J/mol×K	502.95	Joback Method
cpg	324.51	J/mol×K	540.85	Joback Method
cpg	340.68	J/mol×K	578.75	Joback Method
cpg	355.94	J/mol×K	616.65	Joback Method
cpg	370.30	J/mol×K	654.55	Joback Method
cpg	383.78	J/mol×K	692.45	Joback Method

cpg	396.39	J/mol×K	730.35	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=R497475&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume