

Thiazolidine, 2-butyl-

Other names:	2-n-Butylthiazolidine 2-Butylthiazolidine
Inchi:	InChI=1S/C7H15NS/c1-2-3-4-7-8-5-6-9-7/h7-8H,2-6H2,1H3
InchiKey:	BOOIWYNDUXYILL-UHFFFAOYSA-N
Formula:	C7H15NS
SMILES:	CCCCC1NCCS1
Mol. weight [g/mol]:	145.27
CAS:	30188-50-2

Physical Properties

Property code	Value	Unit	Source
gf	172.18	kJ/mol	Joback Method
hf	-44.26	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	44.00	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.839		Crippen Method
mcvol	124.960	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1182.00		NIST Webbook
ripol	1719.00		NIST Webbook
tb	471.22	K	Joback Method
tc	689.05	K	Joback Method
tf	368.03	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.38	J/mol×K	471.22	Joback Method
cpg	279.04	J/mol×K	507.52	Joback Method
cpg	293.88	J/mol×K	543.83	Joback Method
cpg	307.94	J/mol×K	580.13	Joback Method

cpg	321.22	J/mol×K	616.44	Joback Method
cpg	333.77	J/mol×K	652.74	Joback Method
cpg	345.61	J/mol×K	689.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30188502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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