Thiazolidine, 2-pentyl-

Other names: 2-Pentylthiazolidine
Inchi: InChI=1S/C8H17NS/c1-2-3-4-5-8-9-6-7-10-8/h8-9H,2-7H2,1H3
InchiKey: MOVBGBMWKHJQKI-UHFFFAOYSA-N
Formula: C8H17NS
SMILES: CCCCCC1NCCS1
Mol. weight [g/mol]: 159.29
CAS: 41204-65-3

Physical Properties

Property code	Value	Unit	Source
gf	180.60	kJ/mol	Joback Method
hf	-64.90	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.229		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1296.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1344.00		NIST Webbook
ripol	1838.00		NIST Webbook
tb	494.10	K	Joback Method
tc	708.59	K	Joback Method
tf	379.30	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.53	J/mol×K	494.10	Joback Method
cpg	324.19	J/mol×K	529.85	Joback Method
cpg	339.98	J/mol×K	565.60	Joback Method
cpg	354.93	J/mol×K	601.35	Joback Method

cpg	369.07	J/mol×K	637.10	Joback Method
cpg	382.42	J/mol×K	672.84	Joback Method
cpg	395.02	J/mol×K	708.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41204653&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume