

«delta»-Thionodecalactone

Other names:	6-pentyl-tetrahydropyran-2-thione
Inchi:	InChI=1S/C10H18OS/c1-2-3-4-6-9-7-5-8-10(12)11-9/h9H,2-8H2,1H3
InchiKey:	MGGPRZOZXNMQM-Q-UHFFFAOYSA-N
Formula:	C10H18OS
SMILES:	CCCCC1CCCC(=S)O1
Mol. weight [g/mol]:	186.31
CAS:	207669-74-7

Physical Properties

Property code	Value	Unit	Source
gf	62.50	kJ/mol	Joback Method
hf	-212.31	kJ/mol	Joback Method
hfus	27.50	kJ/mol	Joback Method
hvap	50.27	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.463		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
ripol	2361.00		NIST Webbook
ripol	2361.00		NIST Webbook
tb	547.34	K	Joback Method
tc	762.49	K	Joback Method
tf	300.08	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.94	J/mol×K	547.34	Joback Method
cpg	395.90	J/mol×K	583.20	Joback Method
cpg	411.85	J/mol×K	619.06	Joback Method
cpg	426.86	J/mol×K	654.91	Joback Method

cpg	440.95	J/mol×K	690.77	Joback Method
cpg	454.19	J/mol×K	726.63	Joback Method
cpg	466.60	J/mol×K	762.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C207669747&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

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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