1,5-dithiacyclooctane

Inchi: InChI=1S/C7H14S2/c1-2-5-9-7-3-6-8-4-1/h1-7H2
InchiKey: KOZNIBXZFWPVBI-UHFFFAOYSA-N
Formula: C7H14S2
SMILES: C1CCSCCCSC1
Mol. weight [g/mol]: 162.32

Physical Properties

Property code	Value	Unit	Source
gf	83.64	kJ/mol	Joback Method
hf	-41.11	kJ/mol	Joback Method
hfus	5.66	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.637		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
rinpol	1225.00		NIST Webbook
rinpol	1235.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1761.00		NIST Webbook
tb	492.25	K	Joback Method
tc	757.58	K	Joback Method
tf	336.61	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.26	J/mol×K	492.25	Joback Method
cpg	284.92	J/mol×K	536.47	Joback Method
cpg	303.28	J/mol×K	580.69	Joback Method
cpg	320.37	J/mol×K	624.91	Joback Method
cpg	336.21	J/mol×K	669.13	Joback Method
cpg	350.82	J/mol×K	713.35	Joback Method

cpg	364.20	J/mol×K	757.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222365&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

Latest version available from:
https://www.chemeo.com/cid/41-206-7/1-5-dithiacyclooctane.pdf
Generated by Cheméo on 2024-10-12 05:47:49.760791974 +0000 UTC m=+3292932.397761223.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.