

(c-C3H5)2CS

Inchi: InChI=1S/C7H10S/c8-7(5-1-2-5)6-3-4-6/h5-6H,1-4H2
InchiKey: KFENTQQGFOBLHNN-UHFFFAOYSA-N
Formula: C7H10S
SMILES: S=C(C1CC1)C1CC1
Mol. weight [g/mol]: 126.22
CAS: 38381-24-7

Physical Properties

Property code	Value	Unit	Source
affp	904.30	kJ/mol	NIST Webbook
basg	874.50	kJ/mol	NIST Webbook
gf	246.62	kJ/mol	Joback Method
hf	104.29	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	37.73	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.176		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
tb	443.08	K	Joback Method
tc	670.14	K	Joback Method
tf	238.80	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.85	J/molxK	443.08	Joback Method
cpg	215.51	J/molxK	480.92	Joback Method
cpg	228.85	J/molxK	518.77	Joback Method
cpg	240.98	J/molxK	556.61	Joback Method
cpg	252.02	J/molxK	594.45	Joback Method
cpg	262.10	J/molxK	632.30	Joback Method
cpg	271.33	J/molxK	670.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38381247&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

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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