

Mercapto-d

Inchi:	InChI=1S/HS/h1H/i1D
InchiKey:	PXQLVRUNWNTZOS-MICDWDOJSA-N
Formula:	DS
SMILES:	[SH]
Mol. weight [g/mol]:	34.08
CAS:	13780-23-9

Physical Properties

Property code	Value	Unit	Source
gf	30.89	kJ/mol	Joback Method
hf	50.96	kJ/mol	Joback Method
hfus	1.48	kJ/mol	Joback Method
hvap	22.18	kJ/mol	Joback Method
log10ws	-0.34		Crippen Method
logp	0.381		Crippen Method
mvol	25.060	ml/mol	McGowan Method
pc	8116.22	kPa	Joback Method
tb	261.56	K	Joback Method
tc	445.60	K	Joback Method
tf	142.59	K	Joback Method
vc	0.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	20.22	J/mol×K	261.56	Joback Method
cpg	21.57	J/mol×K	292.23	Joback Method
cpg	22.69	J/mol×K	322.91	Joback Method
cpg	23.62	J/mol×K	353.58	Joback Method
cpg	24.36	J/mol×K	384.25	Joback Method
cpg	24.95	J/mol×K	414.93	Joback Method
cpg	25.38	J/mol×K	445.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13780239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	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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