

Cysteine, n-octyl-

Inchi:	InChI=1S/C11H23NO2S/c1-2-3-4-5-6-7-8-12-10(9-15)11(13)14/h10,12,15H,2-9H2,1H3,(
InchiKey:	ODUXJJSEHOSSRB-UHFFFAOYSA-N
Formula:	C11H23NO2S
SMILES:	CCCCCCCCNC(CS)C(=O)O
Mol. weight [g/mol]:	233.37
CAS:	133294-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-107.66	kJ/mol	Joback Method
hf	-448.51	kJ/mol	Joback Method
hfus	35.55	kJ/mol	Joback Method
hvap	76.29	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.320		Crippen Method
mcvol	199.620	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
tb	709.72	K	Joback Method
tc	895.61	K	Joback Method
tf	398.60	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.75	J/molxK	709.72	Joback Method
cpg	572.79	J/molxK	740.70	Joback Method
cpg	585.15	J/molxK	771.68	Joback Method
cpg	596.84	J/molxK	802.67	Joback Method
cpg	607.89	J/molxK	833.65	Joback Method
cpg	618.33	J/molxK	864.63	Joback Method
cpg	628.17	J/molxK	895.61	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C133294141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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