

Thiocyanic acid, octyl ester

Other names:	Octyl thiocyanate 1-Thiocyanatooctane n-Octyl thiocyanate Octyl rhodanate Oktylthiokyanat
Inchi:	InChI=1S/C9H17NS/c1-2-3-4-5-6-7-8-11-9-10/h2-8H2,1H3
InchiKey:	FGVYCHQRRXRDRAR-UHFFFAOYSA-N
Formula:	C9H17NS
SMILES:	CCCCCCCCSC#N
Mol. weight [g/mol]:	171.30
CAS:	19942-78-0

Physical Properties

Property code	Value	Unit	Source
gf	191.20	kJ/mol	Joback Method
hf	-22.34	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.561		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
tb	576.18	K	Joback Method
tc	777.15	K	Joback Method
tf	290.58	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.20	J/molxK	576.18	Joback Method
cpg	379.11	J/molxK	609.68	Joback Method
cpg	391.39	J/molxK	643.17	Joback Method
cpg	403.06	J/molxK	676.67	Joback Method

cpg	414.12	J/mol×K	710.16	Joback Method
cpg	424.59	J/mol×K	743.66	Joback Method
cpg	434.49	J/mol×K	777.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.70	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19942780&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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