Dodecyl thiocyanate

Other names:	n-Dodecyl thiocyanate
	Dodecane, 1-thiocyanato-
	ENT 114
	Lauryl rhodanate
	Lauryl thiocyanate
	Lorol thiocyanate
	LORO
	Thiocyanic acid, dodecyl ester
	Laurylrhodanide
	Laurylthiokyanat
	1-Dodecyl thiocyanate
	NSC 1481
Inchi:	InChI=1S/C13H25NS/c1-2-3-4-5-6-7-8-9-10-11-12-15-13-14/h2-12H2,1H3
InchiKey:	RYZZMYXTNUJGMU-UHFFFAOYSA-N
Formula:	C13H25NS
SMILES:	CCCCCCCCCCCCSC#N
Mol. weight [g/mol]:	227.41
CAS:	765-15-1

Physical Properties

Property code	Value	Unit	Source
gf	224.88	kJ/mol	Joback Method
hf	-104.90	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	61.83	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.122		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
tb	667.70	K	Joback Method
tc	859.10	K	Joback Method
tf	335.66	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.24	J/mol×K	667.70	Joback Method
cpg	582.70	J/mol×K	699.60	Joback Method
cpg	597.39	J/mol×K	731.50	Joback Method
cpg	611.31	J/mol×K	763.40	Joback Method
cpg	624.50	J/mol×K	795.30	Joback Method
cpg	636.98	J/mol×K	827.20	Joback Method
cpg	648.77	J/mol×K	859.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765151&Units=SI

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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