

Phenacyl thiocyanate

Inchi:	InChI=1S/C9H7NOS/c10-7-12-6-9(11)8-4-2-1-3-5-8/h1-5H,6H2
InchiKey:	DLLVIJACDVJDIP-UHFFFAOYSA-N
Formula:	C9H7NOS
SMILES:	N#CSCC(=O)c1ccccc1
Mol. weight [g/mol]:	177.22
CAS:	5399-30-4

Physical Properties

Property code	Value	Unit	Source
gf	174.69	kJ/mol	Joback Method
hf	101.61	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	61.94	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.084		Crippen Method
mcvol	133.210	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	656.73	K	Joback Method
tc	910.29	K	Joback Method
tf	366.93	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.70	J/molxK	656.73	Joback Method
cpg	308.73	J/molxK	698.99	Joback Method
cpg	317.89	J/molxK	741.25	Joback Method
cpg	326.23	J/molxK	783.51	Joback Method
cpg	333.77	J/molxK	825.77	Joback Method
cpg	340.54	J/molxK	868.03	Joback Method
cpg	346.60	J/molxK	910.29	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=C5399304&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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