N,N-Dimethyl phenyl(thioacetamide)

Inchi: InChI=1S/C10H13NS/c1-11(2)10(12)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3
InchiKey: WLOKDAWGDBJTFR-UHFFFAOYSA-N
Formula: C10H13NS
SMILES: CN(C)C(=S)Cc1ccccc1
Mol. weight [g/mol]: 179.28
CAS: 17709-95-4

Physical Properties

Property code	Value	Unit	Source
gf	373.57	kJ/mol	Joback Method
hf	200.83	kJ/mol	Joback Method
hfus	23.32	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.118		Crippen Method
mcvol	150.030	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
tb	537.36	K	Joback Method
tc	766.04	K	Joback Method
tf	295.62	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.29	J/mol×K	537.36	Joback Method
cpg	341.14	J/mol×K	575.47	Joback Method
cpg	354.84	J/mol×K	613.59	Joback Method
cpg	367.47	J/mol×K	651.70	Joback Method
cpg	379.14	J/mol×K	689.81	Joback Method
cpg	389.93	J/mol×K	727.93	Joback Method
cpg	399.94	J/mol×K	766.04	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=C17709954&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