4-(Trifluoromethyl)thiobenzamide

Inchi: InChI=1S/C8H6F3NS/c9-8(10,11)6-3-1-5(2-4-6)7(12)13/h1-4H,(H2,12,13)
InchiKey: IPRFNMJROWWFBH-UHFFFAOYSA-N
Formula: C8H6F3NS
SMILES: NC(=S)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 205.20
CAS: 72505-21-6

Physical Properties

Property code	Value	Unit	Source
gf	-278.82	kJ/mol	Joback Method
hf	-400.18	kJ/mol	Joback Method
hfus	21.75	kJ/mol	Joback Method
hvap	49.96	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.340		Crippen Method
mcvol	127.160	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	551.25	K	Joback Method
tc	781.05	K	Joback Method
tf	340.58	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.65	J/mol×K	551.25	Joback Method
cpg	295.94	J/mol×K	589.55	Joback Method
cpg	305.23	J/mol×K	627.85	Joback Method
cpg	313.64	J/mol×K	666.15	Joback Method
cpg	321.26	J/mol×K	704.45	Joback Method
cpg	328.18	J/mol×K	742.75	Joback Method
cpg	334.50	J/mol×K	781.05	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=C72505216&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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