Benzenecarbothioamide

Other names:	Benzamide, thio-
	Benzothiamide
	Benzothioamide
	Thiobenzamide
	Phenylthioamide
	Tiobenzamide
Inchi:	InChI=1S/C7H7NS/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H2,8,9)
InchiKey:	QIOZLISABUUKJY-UHFFFAOYSA-N
Formula:	C7H7NS
SMILES:	NC(=S)c1ccccc1
Mol. weight [g/mol]:	137.20
CAS:	2227-79-4

Physical Properties

Property code	Value	Unit	Source
chs	-4401.40 ± 1.10	kJ/mol	NIST Webbook
chs	-4390.78 ± 0.99	kJ/mol	NIST Webbook
gf	303.98	kJ/mol	Joback Method
hf	147.80 ± 2.70	kJ/mol	NIST Webbook
hf	131.00 ± 1.30	kJ/mol	NIST Webbook
hfs	33.80 ± 1.10	kJ/mol	NIST Webbook
hfs	44.40 ± 1.50	kJ/mol	NIST Webbook
hfus	17.73	kJ/mol	Joback Method
hsub	97.20 ± 0.60	kJ/mol	NIST Webbook
hsub	97.20 ± 0.60	kJ/mol	NIST Webbook
hsub	103.40 ± 2.20	kJ/mol	NIST Webbook
hvap	50.82	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-2.24		Crippen Method
logp	1.321		Crippen Method
mcvol	107.760	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	528.81	K	Joback Method
tc	785.82	K	Joback Method
tf	312.60	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.99	J/mol×K	528.81	Joback Method
cpg	225.57	J/mol×K	571.65	Joback Method
cpg	235.15	J/mol×K	614.48	Joback Method
cpg	243.82	J/mol×K	657.32	Joback Method
cpg	251.69	J/mol×K	700.15	Joback Method
cpg	258.86	J/mol×K	742.99	Joback Method
cpg	265.42	J/mol×K	785.82	Joback Method
cps	152.80	J/mol×K	298.00	NIST Webbook
hsubt	97.20	kJ/mol	298.15	NIST Webbook
hsubt	103.40 ± 2.20	kJ/mol	289.00	NIST Webbook
ssubt	326.00	J/mol×K	298.15	NIST Webbook

Sources

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=C2227794&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume