

Endo-bicyclo[2.2.1]heptane-2-carbonitrile

Inchi:	InChI=1S/C8H11N/c9-5-8-4-6-1-2-7(8)3-6/h6-8H,1-4H2/t6?,7?,8-/m1/s1
InchiKey:	GAHKEUUHTHVKEA-KAVNDROISA-N
Formula:	C8H11N
SMILES:	N#CC1CC2CCCC1C2
Mol. weight [g/mol]:	121.18
CAS:	3211-87-8

Physical Properties

Property code	Value	Unit	Source
chs	-4740.40 ± 1.50	kJ/mol	NIST Webbook
gf	251.35	kJ/mol	Joback Method
hf	75.53	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	43.57	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.946		Crippen Method
mcvol	103.240	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
ss	224.68	J/mol×K	NIST Webbook
ss	223.80	J/mol×K	NIST Webbook
tb	497.60	K	Joback Method
tc	721.31	K	Joback Method
tf	273.03	K	Joback Method
tt	331.20 ± 0.10	K	NIST Webbook
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.98	J/mol×K	609.45	Joback Method
cpg	270.18	J/mol×K	572.17	Joback Method
cpg	316.31	J/mol×K	721.31	Joback Method
cpg	305.98	J/mol×K	684.02	Joback Method
cpg	294.89	J/mol×K	646.74	Joback Method

cpg	241.64	J/mol×K	497.60	Joback Method
cpg	256.42	J/mol×K	534.88	Joback Method
cps	193.93	J/mol×K	298.15	NIST Webbook
cps	193.89	J/mol×K	298.15	NIST Webbook
hfust	2.96	kJ/mol	331.20	NIST Webbook
hfust	2.25	kJ/mol	177.30	NIST Webbook
hfust	2.96	kJ/mol	331.20	NIST Webbook
sfust	8.94	J/mol×K	331.20	NIST Webbook
sfust	12.70	J/mol×K	177.30	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=C3211878&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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume

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