Exo-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-/m0/s1
InchiKey: GAHKEUUHTHVKEA-RRQHEKLDSA-N
Formula: C8H11N
SMILES: N#CC1CC2CCC1C2
Mol. weight [g/mol]: 121.18
CAS: 3211-90-3

Physical Properties

Property code	Value	Unit	Source
chl	-4739.20 ± 1.30	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	241.70	J/mol×K	NIST Webbook
ss	230.58	J/mol×K	NIST Webbook
tb	497.60	K	Joback Method
tc	721.31	K	Joback Method
tf	299.60	K	NIST Webbook
tt	298.80 ± 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	294.89	J/mol×K	646.74	Joback Method
cpg	305.98	J/mol×K	684.02	Joback Method
cpg	241.64	J/mol×K	497.60	Joback Method
cpg	256.42	J/mol×K	534.88	Joback Method

cpg	270.18	J/mol×K	572.17	Joback Method
cpg	316.31	J/mol×K	721.31	Joback Method
cps	200.00	J/mol×K	285.00	NIST Webbook
cps	200.03	J/mol×K	280.00	NIST Webbook
hfust	2.93	kJ/mol	298.80	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.00	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3211903&Units=SI
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

Legend

chl: Standard liquid 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
ss: Solid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume