Cycloheptyl cyanide

Other names: Cycloheptanecarbonitrile
Inchi: InChI=1S/C8H13N/c9-7-8-5-3-1-2-4-6-8/h8H,1-6H2
InchiKey: UIZRDFICGGONJJ-UHFFFAOYSA-N
Formula: C8H13N
SMILES: N#CC1CCCCCC1
Mol. weight [g/mol]: 123.20
CAS: 32730-85-1

Physical Properties

Property code	Value	Unit	Source
gf	162.01	kJ/mol	Joback Method
hf	4.59	kJ/mol	Joback Method
hfus	7.72	kJ/mol	Joback Method
hvap	44.48	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.480		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	508.34	K	Joback Method
tc	740.26	K	Joback Method
tf	248.77	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.50	J/mol×K	508.34	Joback Method
cpg	270.78	J/mol×K	546.99	Joback Method
cpg	286.10	J/mol×K	585.65	Joback Method
cpg	300.48	J/mol×K	624.30	Joback Method
cpg	313.94	J/mol×K	662.96	Joback Method
cpg	326.50	J/mol×K	701.61	Joback Method
cpg	338.19	J/mol×K	740.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.70	K	1.30	NIST Webbook

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=C32730851&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume