4-Methyl-3-cyclohexene-1-carbonitrile

Inchi: InChI=1S/C8H11N/c1-7-2-4-8(6-9)5-3-7/h2,8H,3-5H2,1H3
InchiKey: WJCYDDFWVABXMW-UHFFFAOYSA-N
Formula: C8H11N
SMILES: CC1=CCC(C#N)CC1
Mol. weight [g/mol]: 121.18
CAS: 6824-60-8

Physical Properties

Property code	Value	Unit	Source
gf	194.44	kJ/mol	Joback Method
hf	57.06	kJ/mol	Joback Method
hfus	10.65	kJ/mol	Joback Method
hvap	45.26	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.256		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	508.21	K	Joback Method
tc	735.02	K	Joback Method
tf	265.57	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.66	J/mol×K	508.21	Joback Method
cpg	251.21	J/mol×K	546.01	Joback Method
cpg	263.98	J/mol×K	583.81	Joback Method
cpg	276.00	J/mol×K	621.62	Joback Method
cpg	287.27	J/mol×K	659.42	Joback Method
cpg	297.84	J/mol×K	697.22	Joback Method
cpg	307.71	J/mol×K	735.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6824608&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

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