Bicyclo[2.2.2]oct-5-ene-2-carbonitrile, 3-methyl-, (1«alpha»,2«alpha»,3«beta»,4«alpha»)-(endo,exo)

Inchi: InChI=1S/C10H15N/b1-7/8-2-4-9(5-3-8)10(7)6-11/h7-10H,2-5H2,1H3/t7-,8?,9?,10+/m1/s

InchiKey: ZFLTZPJOKVUDPQ-WOOKNIGNSA-N

Formula: C10H13N

SMILES: CC1C2CCC(CC2)C1C#N

Mol. weight [g/mol]: 147.22

CAS: 114718-70-6

Physical Properties

Property code	Value	Unit	Source
gf	248.38	kJ/mol	Joback Method
hf	127.00	kJ/mol	NIST Webbook
hfus	17.37	kJ/mol	Joback Method
hvap	47.88	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.582		Crippen Method
mcvol	131.420	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	542.96	K	Joback Method
tc	766.99	K	Joback Method
tf	287.81	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.51	J/mol×K	542.96	Joback Method
cpg	352.31	J/mol×K	580.30	Joback Method
cpg	368.98	J/mol×K	617.64	Joback Method
cpg	384.58	J/mol×K	654.98	Joback Method
cpg	399.16	J/mol×K	692.32	Joback Method
cpg	412.78	J/mol×K	729.66	Joback Method
cpg	425.50	J/mol×K	766.99	Joback Method

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=C114718706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/79-598-2/Bicyclo-2-2-2-oct-5-ene-2-carbonitrile-3-methyl-1-alpha-2-alpha-3-beta-4-alph
Generated by Cheméo on 2024-10-12 09:06:26.640301339 +0000 UTC m=+3304849.277270598.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.