Cinnamonitrile, 2-cyano, trans

Inchi: InChI=1S/C10H6N2/c11-7-3-6-9-4-1-2-5-10(9)8-12/h1-6H/b6-3+
InchiKey: XICDCENQIKYMGT-ZZXKWVIFSA-N
Formula: C10H6N2
SMILES: N#CC=Cc1ccccc1C#N
Mol. weight [g/mol]: 154.17

Physical Properties

Property code	Value	Unit	Source
gf	482.68	kJ/mol	Joback Method
hf	422.31	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	61.71	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.095		Crippen Method
mcvol	126.460	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1531.00		NIST Webbook
tb	668.18	K	Joback Method
tc	916.41	K	Joback Method
tf	366.30	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.81	J/mol×K	668.18	Joback Method
cpg	290.57	J/mol×K	709.55	Joback Method
cpg	298.63	J/mol×K	750.92	Joback Method
cpg	306.07	J/mol×K	792.29	Joback Method
cpg	312.93	J/mol×K	833.66	Joback Method
cpg	319.29	J/mol×K	875.03	Joback Method
cpg	325.21	J/mol×K	916.41	Joback Method

Sources

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=R503778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume