2-Propenenitrile, 3-phenyl-, (E)-

Other names:	trans-Cinnamonitrile (E)-Cinnamonitrile (E)-3-Phenylacrylonitrile trans-«beta»-Phenylacrylonitrile trans-3-Phenylpropenonitrile Cinnamonitrile, (E)- (E)-3-Phenylpropenenitrile (E)-3-Phenylprop-2-enenitrile 2-Propenenitrile, 3-phenyl-, (2E)- NSC 77496 trans-3-Phenyl-2-propenenitrile cinnamonitrile
Inchi:	InChI=1S/C9H7N/c10-8-4-7-9-5-2-1-3-6-9/h1-7H/b7-4+
InchiKey:	ZWKNLRXFUTWSOY-QPJJXVBHSA-N
Formula:	C9H7N
SMILES:	N#CC=Cc1ccccc1
Mol. weight [g/mol]:	129.16
CAS:	1885-38-7

Physical Properties

Property code	Value	Unit	Source
gf	350.71	kJ/mol	Joback Method
hf	289.54	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.223		Crippen Method
mcvol	110.990	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1301.10		NIST Webbook
rinpol	1301.10		NIST Webbook
tb	527.70	K	NIST Webbook
tc	776.63	K	Joback Method
tf	277.52	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.13	J/mol×K	538.24	Joback Method
cpg	235.97	J/mol×K	577.97	Joback Method
cpg	245.97	J/mol×K	617.70	Joback Method
cpg	255.18	J/mol×K	657.44	Joback Method
cpg	263.67	J/mol×K	697.17	Joback Method
cpg	271.49	J/mol×K	736.90	Joback Method
cpg	278.72	J/mol×K	776.63	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=C1885387&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume