Geranonitrile # 3

Other names:	Geranonitrile # 2
	Geranonitrile, # 1
	Geranyl nitrile
	2-Geranonitrile
	Geranonitrile
	(E)-3,7-dimethyl-2,6-octadienenitrile
Inchi:	InChI=1S/C10H15N/c1-9(2)5-4-6-10(3)7-8-11/h5,7H,4,6H2,1-3H3/b10-7+
InchiKey:	HLCSDJLATUNSSI-JXMROGBWSA-N
Formula:	C10H15N
SMILES:	CC(C)=CCCC(C)=CC#N
Mol. weight [g/mol]:	149.23
CAS:	5585-39-7

Physical Properties

Property code	Value	Unit	Source
gf	309.84	kJ/mol	Joback Method
hf	130.01	kJ/mol	Joback Method
hfus	20.95	kJ/mol	Joback Method
hvap	48.41	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.203		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1228.30		NIST Webbook
rinpol	1196.40		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1723.00		NIST Webbook
tb	538.36	K	Joback Method
tc	742.94	K	Joback Method
tf	229.37	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.39	J/mol×K	538.36	Joback Method
cpg	335.31	J/mol×K	572.46	Joback Method
cpg	347.49	J/mol×K	606.55	Joback Method
cpg	358.97	J/mol×K	640.65	Joback Method
cpg	369.81	J/mol×K	674.75	Joback Method
cpg	380.06	J/mol×K	708.84	Joback Method
cpg	389.75	J/mol×K	742.94	Joback Method

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=C5585397&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume