1,3,5-Pentanetricarbonitrile, 3-phenyl

Inchi: InChI=1S/C14H13N3/c15-10-4-8-14(12-17,9-5-11-16)13-6-2-1-3-7-13/h1-3,6-7H,4-5,8-9H
InchiKey: KVDYEBISIZWSRT-UHFFFAOYSA-N
Formula: C14H13N3
SMILES: N#CCCC(C#N)(CCC#N)c1ccccc1
Mol. weight [g/mol]: 223.27
CAS: 16320-20-0

Physical Properties

Property code	Value	Unit	Source
gf	581.79	kJ/mol	Joback Method
hf	390.13	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	79.17	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.056		Crippen Method
mcvol	188.500	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
tb	849.41	K	Joback Method
tc	1091.29	K	Joback Method
tf	471.35	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.08	J/mol×K	849.41	Joback Method
cpg	530.81	J/mol×K	889.72	Joback Method
cpg	539.81	J/mol×K	930.04	Joback Method
cpg	548.18	J/mol×K	970.35	Joback Method
cpg	556.01	J/mol×K	1010.67	Joback Method
cpg	563.38	J/mol×K	1050.98	Joback Method
cpg	570.40	J/mol×K	1091.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16320200&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

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