Pentamethylphenylacetonitrile

Inchi:	InChI=1S/C13H17N/c1-8-9(2)11(4)13(6-7-14)12(5)10(8)3/h6H2,1-5H3
InchiKey:	FJHYQRAQLGAUPF-UHFFFAOYSA-N
Formula:	C13H17N
SMILES:	Cc1c(C)c(C)c(CC#N)c(C)c1C
Mol. weight [g/mol]:	187.28
CAS:	34688-70-5

Physical Properties

Property code	Value	Unit	Source
gf	256.02	kJ/mol	Joback Method
hf	32.41	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	60.60	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.295		Crippen Method
mcvol	171.650	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
tb	650.50	K	Joback Method
tc	866.87	K	Joback Method
tf	390.28	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.39	J/mol×K	650.50	Joback Method
cpg	441.20	J/mol×K	686.56	Joback Method
cpg	454.29	J/mol×K	722.62	Joback Method
cpg	466.70	J/mol×K	758.69	Joback Method
cpg	478.43	J/mol×K	794.75	Joback Method
cpg	489.49	J/mol×K	830.81	Joback Method
cpg	499.89	J/mol×K	866.87	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=C34688705&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

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