2-Phenylvaleronitrile

Other names: Benzeneacetonitrile, «alpha»-propyl-
Inchi: InChI=1S/C11H13N/c1-2-6-11(9-12)10-7-4-3-5-8-10/h3-5,7-8,11H,2,6H2,1H3
InchiKey: VIUPTAFHLRBHBO-UHFFFAOYSA-N
Formula: C11H13N
SMILES: CCCC(C#N)c1ccccc1
Mol. weight [g/mol]: 159.23
CAS: 5558-78-1

Physical Properties

Property code	Value	Unit	Source
gf	284.89	kJ/mol	Joback Method
hf	125.76	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.094		Crippen Method
mcvol	143.470	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	579.40	K	Joback Method
tc	803.45	K	Joback Method
tf	290.14	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.80	J/mol×K	579.40	Joback Method
cpg	348.53	J/mol×K	616.74	Joback Method
cpg	361.37	J/mol×K	654.08	Joback Method
cpg	373.35	J/mol×K	691.43	Joback Method
cpg	384.52	J/mol×K	728.77	Joback Method
cpg	394.93	J/mol×K	766.11	Joback Method
cpg	404.60	J/mol×K	803.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.70	K	1.70	NIST Webbook
tbrp	399.50 ± 1.50	K	1.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5558781&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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