Butyronitrile, 2-ethyl-2-phenyl-

Other names: 2-Ethyl-2-phenylbutyronitrile
Inchi: InChI=1S/C12H15N/c1-3-12(4-2,10-13)11-8-6-5-7-9-11/h5-9H,3-4H2,1-2H3
InchiKey: NIWOFSGCBJZYJQ-UHFFFAOYSA-N
Formula: C12H15N
SMILES: CCC(C#N)(CC)c1ccccc1
Mol. weight [g/mol]: 173.25
CAS: 5336-57-2

Physical Properties

Property code	Value	Unit	Source
gf	298.59	kJ/mol	Joback Method
hf	101.65	kJ/mol	Joback Method
hfus	14.97	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.268		Crippen Method
mcvol	157.560	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
tb	599.49	K	Joback Method
tc	828.21	K	Joback Method
tf	318.83	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.46	J/mol×K	599.49	Joback Method
cpg	400.34	J/mol×K	637.61	Joback Method
cpg	414.13	J/mol×K	675.73	Joback Method
cpg	426.90	J/mol×K	713.85	Joback Method
cpg	438.73	J/mol×K	751.97	Joback Method
cpg	449.70	J/mol×K	790.09	Joback Method
cpg	459.87	J/mol×K	828.21	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=C5336572&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