2,2-DIPHENYLPROPIONITRILE

Other names: 2,2-diphenylpropiononitrile
Benzeneacetonitrile, «alpha»-methyl-«alpha»-phenyl-«alpha»,«alpha»-Diphenylpropionitrile
Inchi: InChI=1S/C15H13N/c1-15(12-16,13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-11H,1H3
InchiKey: DPVHBXFSKLKYIQ-UHFFFAOYSA-N
Formula: C15H13N
SMILES: CC(C#N)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 207.28

Physical Properties

Property code	Value	Unit	Source
af	0.4651		Cheméo Relay (1.0)
hf	296.01	kJ/mol	Cheméo Relay (1.0)
hfus	16.78	kJ/mol	Joback Method
hvap	79.04	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-4.69		Cheméo Relay (1.0)
logp	3.516		Crippen Method
mcvol	176.070	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
tb	572.78	K	Cheméo Relay (1.0)
tc	848.67	K	Cheméo Relay (1.0)
tf	365.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.88	J/mol×K	694.81	Joback Method
cpg	468.85	J/mol×K	738.54	Joback Method
cpg	482.43	J/mol×K	782.26	Joback Method
cpg	494.74	J/mol×K	825.99	Joback Method
cpg	505.94	J/mol×K	869.71	Joback Method
cpg	516.16	J/mol×K	913.44	Joback Method
cpg	525.56	J/mol×K	957.17	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5558678&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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