2,2-Diphenylpropionitrile

Other names:	«alpha»,«alpha»-Diphenylpropionitrile Benzeneacetonitrile, «alpha»-methyl-«alpha»-phenyl- 2,2-diphenylpropiononitrile
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]:	207.27
CAS:	5558-67-8

Physical Properties

Property code	Value	Unit	Source
gf	436.26	kJ/mol	Joback Method
hf	276.26	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.516		Crippen Method
mcvol	176.070	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
tb	694.81	K	Joback Method
tc	957.17	K	Joback Method
tf	379.06	K	Joback Method
vc	0.674	m3/kmol	Joback Method

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

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=C5558678&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