Benzeneacetonitrile, «alpha»-(phenylmethylene)-

Other names: Acrylonitrile, 2,3-diphenyl-
«alpha»-Cyanostilbene
«alpha»-Phenylcinnamonitrile
«alpha»-Stilbenecarbonitrile
Benzylidenephenylacetonitrile
Cinnamonitrile, «alpha»-phenyl-
Stilbene, «alpha»-cyano-
2,3-Diphenylacrilonitrile
2,3-Diphenylacrylonitrile
«alpha»,«beta»-Diphenyl-«alpha»-cyanoethylene
«alpha»,«beta»-Diphenylacrylonitrile
USAF A-9789
Benzal-(benzyl-cyanid)
F 2387
2,3-Diphenyl-2-propenenitrile
NSC 12489
NSC 2018

Inchi: InChI=1S/C15H11N/c16-12-15(14-9-5-2-6-10-14)11-13-7-3-1-4-8-13/h1-11H/b15-11+

InchiKey: VFOKYTYWXOYPOX-RVDMUPIBSA-N

Formula: C15H11N

SMILES: N#CC(=Cc1ccccc1)c1ccccc1

Mol. weight [g/mol]: 205.25

CAS: 2510-95-4

Physical Properties

Property code	Value	Unit	Source
chs	-7827.00	kJ/mol	NIST Webbook
chs	-7831.00	kJ/mol	NIST Webbook
gf	505.09	kJ/mol	Joback Method
hf	392.44	kJ/mol	Joback Method
hfs	353.00	kJ/mol	NIST Webbook
hfs	352.00	kJ/mol	NIST Webbook
hfus	23.09	kJ/mol	Joback Method
hvap	64.05	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.751		Crippen Method
mcvol	171.770	ml/mol	McGowan Method

pc	2592.49	kPa	Joback Method
tb	702.08	K	Joback Method
tc	964.16	K	Joback Method
tf	357.60	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.10	J/mol×K	702.08	Joback Method
cpg	441.05	J/mol×K	745.76	Joback Method
cpg	453.76	J/mol×K	789.44	Joback Method
cpg	465.35	J/mol×K	833.12	Joback Method
cpg	475.97	J/mol×K	876.80	Joback Method
cpg	485.74	J/mol×K	920.48	Joback Method
cpg	494.79	J/mol×K	964.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2510954&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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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