Malononitrile, benzyl 4-bromophenyldiazenyl-

Other names: N-Bromophenyl-N'-(1,1-dicyano-2-phenyl-ethyl)-diazene
Inchi: InChI=1S/C16H11BrN4/c17-14-6-8-15(9-7-14)20-21-16(11-18,12-19)10-13-4-2-1-3-5-13/
InchiKey: SFPMXPDHZDFXNM-UHFFFAOYSA-N
Formula: C16H11BrN4
SMILES: N#CC(C#N)(Cc1ccccc1)N=Nc1ccc(Br)cc1
Mol. weight [g/mol]: 339.19
CAS: 64710-74-3

Physical Properties

Property code	Value	Unit	Source
hf	482.58	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.561		Crippen Method
mcvol	224.700	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
tb	1040.11	K	Joback Method
tc	1324.00	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64710743&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

hf: Enthalpy of formation 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