Benzene, 1,3-bis(1-isocyanato-1-methylethyl)-

Other names: 1,3-bis(1-isocyanato-1-methylethyl)benzene
Inchi: InChI=1S/C14H16N2O2/c1-13(2,15-9-17)11-6-5-7-12(8-11)14(3,4)16-10-18/h5-8H,1-4H3
InchiKey: AZYRZNIYJDKRHO-UHFFFAOYSA-N
Formula: C14H16N2O2
SMILES: CC(C)(N=C=O)c1cccc(C(C)(C)N=C=O)c1
Mol. weight [g/mol]: 244.29
CAS: 2778-42-9

Physical Properties

Property code	Value	Unit	Source
hf	-135.55	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-12.08		Crippen Method
logp	2.828		Crippen Method
mcvol	198.860	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	678.26	K	Joback Method
tc	909.46	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	464.00	J/mol×K	333.00	NIST Webbook
hvapt	65.20	kJ/mol	362.00	NIST Webbook

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=C2778429&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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