1,1'-(M-PHENYLENE)BIS(ISOPROPYL ISOCYANATE)

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

Physical Properties

Property code	Value	Unit	Source
hvap	71.04	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
logp	2.828		Crippen Method
mcvol	198.860	ml/mol	McGowan Method
tf	351.17	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2778429&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpl:	Liquid phase heat capacity
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point