

N,N,N',N'-Tetraethyl isophthalamide

Inchi:
InchiKey:
Formula:
SMILES:
Mol. weight [g/mol]:

InChI=1S/C16H24N2O2/c1-5-17(6-2)15(19)13-10-9-11-14(12-13)16(20)18(7-3)8-4/h9-12
GZWCNZTWDVSL-UHFFFAOYSA-N
C16H24N2O2
CCN(CC)C(=O)c1cccc(C(=O)N(CC)CC)c1
276.38

Physical Properties

Property code	Value	Unit	Source
hf	-382.93	kJ/mol	Cheméo Relay (1.0)
hfus	40.09	kJ/mol	Joback Method
hvap	81.28	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-3.34		Cheméo Relay (1.0)
logp	2.651		Crippen Method
mcvol	235.640	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
tb	608.58	K	Cheméo Relay (1.0)
tc	835.70	K	Cheméo Relay (1.0)
tf	345.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.25	J/mol×K	729.76	Joback Method
cpg	689.33	J/mol×K	763.14	Joback Method
cpg	704.40	J/mol×K	796.52	Joback Method
cpg	718.51	J/mol×K	829.90	Joback Method
cpg	731.70	J/mol×K	863.28	Joback Method
cpg	744.03	J/mol×K	896.66	Joback Method
cpg	755.55	J/mol×K	930.04	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13698878&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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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