

N,N-Diisopropylbenzamide

Inchi:	InChI=1S/C13H19NO/c1-10(2)14(11(3)4)13(15)12-8-6-5-7-9-12/h5-11H,1-4H3
InchiKey:	UYXMMJJPYFKRKKM-UHFFFAOYSA-N
Formula:	C13H19NO
SMILES:	CC(C)N(C(=O)c1ccccc1)C(C)C
Mol. weight [g/mol]:	205.30
CAS:	20383-28-2

Physical Properties

Property code	Value	Unit	Source
gf	147.97	kJ/mol	Joback Method
hf	-130.73	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.946		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1524.00		NIST Webbook
rinpol	1524.00		NIST Webbook
tb	588.95	K	Joback Method
tc	799.49	K	Joback Method
tf	315.09	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.53	J/molxK	588.95	Joback Method
cpg	471.93	J/molxK	624.04	Joback Method
cpg	488.23	J/molxK	659.13	Joback Method
cpg	503.48	J/molxK	694.22	Joback Method
cpg	517.73	J/molxK	729.31	Joback Method
cpg	531.03	J/molxK	764.40	Joback Method
cpg	543.44	J/molxK	799.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.00 ± 2.00	K	2.40	NIST Webbook

Sources

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=C20383282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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