

N,N-DIBENZOYLMETHYLAMINE

Other names:	N,N-Dibenzoylmethylamin N-benzoyl-N-methylbenzamide
Inchi:	InChI=1S/C15H13NO2/c1-16(14(17)12-8-4-2-5-9-12)15(18)13-10-6-3-7-11-13/h2-11H,1H
InchiKey:	ALISWIYMUUVXSIG-UHFFFAOYSA-N
Formula:	C15H13NO2
SMILES:	CN(C(=O)c1ccccc1)C(=O)c1ccccc1
Mol. weight [g/mol]:	239.27

Physical Properties

Property code	Value	Unit	Source
af	0.6092		Cheméo Relay (1.0)
gf	153.18	kJ/mol	Joback Method
hf	-137.26	kJ/mol	Cheméo Relay (1.0)
hfus	28.91	kJ/mol	Joback Method
hsub	120.10 ± 0.40	kJ/mol	NIST Webbook
hvap	87.75	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-3.18		Cheméo Relay (1.0)
logp	2.599		Crippen Method
mcvol	187.810	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	617.26	K	Cheméo Relay (1.0)
tc	897.23	K	Cheméo Relay (1.0)
tf	376.58	K	Cheméo Relay (1.0)
vc	0.694	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.74	J/mol×K	716.14	Joback Method
cpg	509.17	J/mol×K	756.64	Joback Method
cpg	522.31	J/mol×K	797.15	Joback Method
cpg	534.27	J/mol×K	837.65	Joback Method
cpg	545.14	J/mol×K	878.15	Joback Method

cpg	555.01	J/mol×K	918.65	Joback Method
cpg	563.98	J/mol×K	959.16	Joback Method
hsubt	116.80 ± 0.40	kJ/mol	257.50	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23825323&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

Legend

af:	Acentric Factor
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
vc:	Critical Volume

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