

3-BENZOYL-1,1-DIETHYLUREA

Other names:	N-benzoyl-N',N'-diethylurea
Inchi:	InChI=1S/C12H16N2O2/c1-3-14(4-2)12(16)13-11(15)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H1
InchiKey:	XL MOMZF NQYZDGE-UHFFFAOYSA-N
Formula:	C12H16N2O2
SMILES:	CCN(CC)C(=O)NC(=O)c1ccccc1
Mol. weight [g/mol]:	220.27

Physical Properties

Property code	Value	Unit	Source
af	0.6695		Cheméo Relay (1.0)
hf	-335.00	kJ/mol	Cheméo Relay (1.0)
hfus	32.19	kJ/mol	Joback Method
hsub	132.20 ± 2.80	kJ/mol	NIST Webbook
hvap	86.73	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	1.878		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	579.71	K	Cheméo Relay (1.0)
tc	827.97	K	Cheméo Relay (1.0)
tf	392.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.64	J/mol×K	670.99	Joback Method
cpg	489.61	J/mol×K	706.35	Joback Method
cpg	502.61	J/mol×K	741.71	Joback Method
cpg	514.70	J/mol×K	777.06	Joback Method
cpg	525.91	J/mol×K	812.42	Joback Method
cpg	536.30	J/mol×K	847.78	Joback Method
cpg	545.92	J/mol×K	883.14	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C58328351&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):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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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