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,3-4H2,1-2H
InchiKey: XLMOMZFNQYZDGE-UHFFFAOYSA-N
Formula: C12H16N2O2
SMILES: CCN(CC)C(=O)NC(=O)c1ccccc1
Mol. weight [g/mol]: 220.27
CAS: 58328-35-1

Physical Properties

Property code	Value	Unit	Source
gf	104.90	kJ/mol	Joback Method
hf	-158.64	kJ/mol	Joback Method
hfus	32.19	kJ/mol	Joback Method
hsub	132.20 ± 2.80	kJ/mol	NIST Webbook
hvap	66.55	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.878		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	670.99	K	Joback Method
tc	883.14	K	Joback Method
tf	436.41	K	Joback Method
vc	0.664	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58328351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume