Rebemide

Other names:	Benzamide, N,N-diethyl-
	Benzoic acid diethylamide
	Benzoic acid N,N-diethylamide
	Benzoyldiethylamine
	N,N-Diethylbenzamide
	R 2
	Rebemid
	R 2 (insect repellant)
	REP
	NSC 16060
Inchi:	InChI=1S/C11H15NO/c1-3-12(4-2)11(13)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey:	JLNGEXDJAQASHD-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CCN(CC)C(=O)c1ccccc1
Mol. weight [g/mol]:	177.24
CAS:	1696-17-9

Physical Properties

Property code	Value	Unit	Source
gf	136.01	kJ/mol	Joback Method
hf	-78.89	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hsub	91.40 ± 3.20	kJ/mol	NIST Webbook
hvap	51.14	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.169		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
tb	544.07	K	Joback Method
tc	752.53	K	Joback Method
tf	322.55	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.53	J/mol×K	683.04	Joback Method
cpg	424.39	J/mol×K	717.79	Joback Method
cpg	356.38	J/mol×K	544.07	Joback Method
cpg	371.81	J/mol×K	578.81	Joback Method
cpg	386.29	J/mol×K	613.56	Joback Method
cpg	399.85	J/mol×K	648.30	Joback Method
cpg	435.45	J/mol×K	752.53	Joback Method
hvapt	56.50	kJ/mol	388.00	NIST Webbook
hvapt	53.20	kJ/mol	389.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1696179&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
hvapt: Enthalpy of vaporization at a given temperature
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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume