

BENZAMIDE, N-ETHYL-

Other names:	N-Ethylbenzamide
Inchi:	InChI=1S/C9H11NO/c1-2-10-9(11)8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H,10,11)
InchiKey:	SDIDYFBTIZOPLA-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CCNC(=O)c1ccccc1
Mol. weight [g/mol]:	149.19

Physical Properties

Property code	Value	Unit	Source
af	0.4999		Cheméo Relay (1.0)
gf	97.78	kJ/mol	Joback Method
hf	-135.31	kJ/mol	Cheméo Relay (1.0)
hfus	19.81	kJ/mol	Joback Method
hvap	67.24	kJ/mol	Cheméo Relay (1.0)
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-1.84		Cheméo Relay (1.0)
logp	1.436		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	572.00 ± 1.00	K	NIST Webbook
tc	747.86	K	Cheméo Relay (1.0)
tf	343.50 ± 0.50	K	NIST Webbook
vc	0.454	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.38	J/mol×K	536.04	Joback Method
cpg	291.41	J/mol×K	572.52	Joback Method
cpg	303.61	J/mol×K	609.00	Joback Method
cpg	315.00	J/mol×K	645.47	Joback Method
cpg	325.61	J/mol×K	681.95	Joback Method
cpg	335.50	J/mol×K	718.43	Joback Method
cpg	344.69	J/mol×K	754.91	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C614175&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
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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