Pheneturide

Other names:	Benzeneacetamide, N-(aminocarbonyl)-«alpha»-ethyl-
	Urea, (2-phenylbutyryl)-
	Benuride
	Ethylphenacemide
	1-((Ethyl)phenylacetyl)urea
	Lircapyl
	M 551
	Phenuride
	N-(«alpha»-Phenylbutyryl)urea
	2-Phenylbutyrylurea
	Phenylethylacetylurea
	Phenylethylacetyluree
	S 46
	EPA
	PBU
Inchi:	InChI=1S/C11H14N2O2/c1-2-9(10(14)13-11(12)15)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H3,1
InchiKey:	AJOQSQHYDOFIOX-UHFFFAOYSA-N
Formula:	C11H14N2O2
SMILES:	CCC(C(=O)NC(N)=O)c1ccccc1
Mol. weight [g/mol]:	206.24
CAS:	90-49-3

Physical Properties

Property code	Value	Unit	Source
gf	49.71	kJ/mol	Joback Method
hf	-177.02	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	72.54	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.375		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
tb	707.76	K	Joback Method
tc	937.06	K	Joback Method
tf	460.93	K	Joback Method

vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.15	J/mol×K	707.76	Joback Method
cpg	458.69	J/mol×K	745.98	Joback Method
cpg	470.26	J/mol×K	784.19	Joback Method
cpg	480.90	J/mol×K	822.41	Joback Method
cpg	490.68	J/mol×K	860.62	Joback Method
cpg	499.63	J/mol×K	898.84	Joback Method
cpg	507.82	J/mol×K	937.06	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90493&Units=SI

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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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