

Benzeneacetamide, «alpha»-ethyl-

Other names:	Butyramide, 2-phenyl- «alpha»-Phenylbutyramide «alpha»-Toluamide, «alpha»-ethyl- Eusterol Geriapan Geristerol Hypoesterol Lipilisol Nivonorm Normosterolo Phenetamid Phenetamide Phenexan Phenylethylacetamide Redusterol Substerina TH 4128 2-Phenylbutanamide 2-Phenylbutyramide NSC 1861
Inchi:	InChI=1S/C10H13NO/c1-2-9(10(11)12)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H2,11,12)
InchiKey:	UNFGQCCHVMMMRF-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CCC(C(N)=O)c1ccccc1
Mol. weight [g/mol]:	163.22
CAS:	90-26-6

Physical Properties

Property code	Value	Unit	Source
gf	80.82	kJ/mol	Joback Method
hf	-97.27	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.666		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method

ripol	2600.00		NIST Webbook
tb	580.84	K	Joback Method
tc	809.80	K	Joback Method
tf	347.07	K	Joback Method
vc	0.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.33	J/mol×K	580.84	Joback Method
cpg	348.27	J/mol×K	619.00	Joback Method
cpg	361.25	J/mol×K	657.16	Joback Method
cpg	373.31	J/mol×K	695.32	Joback Method
cpg	384.51	J/mol×K	733.48	Joback Method
cpg	394.88	J/mol×K	771.64	Joback Method
cpg	404.47	J/mol×K	809.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90266&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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