Benzeneacetamide, N-(aminocarbonyl)-

Other names:

Benzeneacetamide, N-(aminocarbonyl)-
Urea, (phenylacetyl)-
«alpha»-Phenylacetylurea
(Phenylacetyl)urea
Cetylureum
Epiclase
Fenacemid
Fenurea
Fenurone
Phacetur
Phenacalum
Phenacetur
Phenacetylcarbamide
Phenacetylurea
Phenicarb
Phenuron
Phenurone
Phenutal
A-1348
Acetylureum
Carbanmide
Comitiadone
Efron
Epheron
Felurea
Fenacemide
Fenacetamide
Fenacetil-Karbamide
Fenilep
Fenised
Fenostenyl
Fenural
Fenytan
Neophedan
Neophenal
Phenacereum
Phenarone
Phenyrit
Phetylureum
Trioxanona

	N-(Aminocarbonyl)benzeneacetamide
	Eferon
	Fenylacetylmocovina
	Phenylacetyluree
	NSC 39458
Inchi:	InChI=1S/C9H10N2O2/c10-9(13)11-8(12)6-7-4-2-1-3-5-7/h1-5H,6H2,(H3,10,11,12,13)
InchiKey:	XPFRXWCVYUEORT-UHFFFAOYSA-N
Formula:	C9H10N2O2
SMILES:	NC(=O)NC(=O)Cc1ccccc1
Mol. weight [g/mol]:	178.19

Physical Properties

Property code	Value	Unit	Source
hf	-339.56	kJ/mol	Cheméo Relay (1.0)
hfus	26.60	kJ/mol	Joback Method
hvap	84.37	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-1.56		Cheméo Relay (1.0)
logp	0.424		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1473.00		NIST Webbook
tb	563.94	K	Cheméo Relay (1.0)
tf	420.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.05	J/mol×K	662.44	Joback Method
cpg	357.11	J/mol×K	701.38	Joback Method
cpg	367.29	J/mol×K	740.33	Joback Method
cpg	376.63	J/mol×K	779.27	Joback Method
cpg	385.19	J/mol×K	818.22	Joback Method
cpg	393.01	J/mol×K	857.16	Joback Method
cpg	400.12	J/mol×K	896.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63989&Units=SI
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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