L-Cysteine, N-acetyl-

Other names:

Acetein
Acetylcysteine
Airbron
Broncholysin
Brunac
Cysteine, N-acetyl-, L-
Fabrol
Fluatox
Fluimicil Infantil
Fluimucetin
Fluimucil
Flumucetin
Fluprowit
Inspir
L-Acetylcysteine
L-«alpha»-Acetamido-«beta»-mercaptopropionic acid
L-Â«alphaÂ»-Acetamido-Â«betaÂ»-mercaptopropionic acid
Lysomucil
Mercapturic acid
Mercapturic acid, (R)-
Muco sanigen
Mucocedyl
Mucofilin
Mucolator
Mucolyticum
Mucolyticum Lappe
Mucolytikum Lappe
Mucomyst
Mucosolvin
Mucret
N-Acetyl-L-cysteine
N-Acetylcysteine
NAC
NAC-TB
NSC 111180
Neo-fluimucil
Parvolex
Respaire
Tixair

Inchi: InChI=1S/C5H9NO3S/c1-3(7)6-4(2-10)5(8)9/h4,10H,2H2,1H3,(H,6,7)(H,8,9)

InchiKey:	PWKSKIMOESPYIA-UHFFFAOYSA-N
Formula:	C5H9NO3S
SMILES:	CC(=O)NC(CS)C(=O)O
Mol. weight [g/mol]:	163.19
CAS:	616-91-1

Physical Properties

Property code	Value	Unit	Source
gf	-287.10	kJ/mol	Joback Method
hf	-437.25	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid
hfus	32.10	kJ/mol	Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds
hvap	69.68	kJ/mol	Joback Method
log10ws	-0.16		Crippen Method
logp	-0.495		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	626.31	K	Joback Method
tc	830.53	K	Joback Method
tf	380.91	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.92	J/mol×K	626.31	Joback Method
cpg	282.74	J/mol×K	660.35	Joback Method
cpg	290.07	J/mol×K	694.38	Joback Method

cpg	296.94	J/mol×K	728.42	Joback Method
cpg	303.37	J/mol×K	762.46	Joback Method
cpg	309.36	J/mol×K	796.50	Joback Method
cpg	314.92	J/mol×K	830.53	Joback Method

Sources

Synthesis and thermodynamics studies of ionic liquid 1-methyl-3-pentylimidazolium bromide ([C5MIM][Br]) with amino acids (L-cysteine and N-acetyl-L-cysteine) at different temperatures:	https://www.doi.org/10.1016/j.jct.2017.03.040
Solubilities of pharmaceutical and bioactive compounds in ionic liquids:	https://www.doi.org/10.1016/j.fluid.2015.03.053
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of pharmaceutical compounds in ionic liquidsAna:	https://www.doi.org/10.1016/j.fluid.2013.07.020
Experimental and computational study on the energetics of N-acetyl-L-cysteine:	https://www.doi.org/10.1016/j.jct.2013.08.026
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds:	https://www.doi.org/10.1016/j.fluid.2014.10.033
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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