Acetylcysteine

Other names:
Acetein
Airbron
Broncholysin
Brunac
Cysteine, N-acetyl-, L-
Fabrol
Fluatox
Fluimicil Infantil
Fluimucetin
Fluimucil
Flumucetin
Fluprowit
Inspir
L-Acetylcysteine
L-«alpha»-Acetamido-«beta»-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)/t4-/m0/s1

InchiKey: PWKSKIMOESPYIA-UHFFFAOYSA-N

Formula: C5H9NO3S

SMILES: CC(=O)NC(CS)C(=O)O
Mol. weight [g/mol]: 163.20

Physical Properties

Property code	Value	Unit	Source
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
hfus	32.10	kJ/mol	Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid
hvap	90.60	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-0.54		Cheméo Relay (1.0)
logp	-0.495		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	545.59	K	Cheméo Relay (1.0)
tf	393.71	K	Cheméo Relay (1.0)

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616911&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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
Experimental and computational study on the energetics of Crippen Method:	https://www.doi.org/10.1016/j.jct.2013.08.026
Solubility of pharmaceutical compounds in ionic liquidsAna:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://www.doi.org/10.1016/j.fluid.2013.07.020
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
	https://www.doi.org/10.1016/j.fluid.2015.03.053

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point