Acetic acid, [3-(2-cyanoethyl)ureido]-, ethyl ester

Inchi: InChI=1S/C8H13N3O3/c1-2-14-7(12)6-11-8(13)10-5-3-4-9/h2-3,5-6H2,1H3,(H2,10,11,13

InchiKey: IGKSODBCEFQNCG-UHFFFAOYSA-N

Formula: C8H13N3O3

SMILES: CCOC(=O)CNC(=O)NCCC#N

Mol. weight [g/mol]: 199.21

CAS: 90641-79-5

Physical Properties

Property code	Value	Unit	Source
gf	-34.40	kJ/mol	Joback Method
hf	-294.01	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	72.65	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	-0.238		Crippen Method
mcvol	153.930	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	715.02	K	Joback Method
tc	916.49	K	Joback Method
tf	472.32	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.81	J/mol×K	715.02	Joback Method
cpg	424.60	J/mol×K	748.60	Joback Method
cpg	433.78	J/mol×K	782.18	Joback Method
cpg	442.35	J/mol×K	815.75	Joback Method
cpg	450.32	J/mol×K	849.33	Joback Method
cpg	457.69	J/mol×K	882.91	Joback Method
cpg	464.48	J/mol×K	916.49	Joback Method

Sources

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=C90641795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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