Acetic acid, (3-methylureido)-, ethyl ester

Inchi: InChI=1S/C6H12N2O3/c1-3-11-5(9)4-8-6(10)7-2/h3-4H2,1-2H3,(H2,7,8,10)
InchiKey: DINZGLVSODXPKH-UHFFFAOYSA-N
Formula: C6H12N2O3
SMILES: CCOC(=O)CNC(=O)NC
Mol. weight [g/mol]: 160.17
CAS: 7150-62-1

Physical Properties

Property code	Value	Unit	Source
gf	-184.42	kJ/mol	Joback Method
hf	-417.61	kJ/mol	Joback Method
hfus	25.88	kJ/mol	Joback Method
hvap	57.72	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	-0.522		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	567.18	K	Joback Method
tc	759.54	K	Joback Method
tf	384.79	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.18	J/mol×K	567.18	Joback Method
cpg	310.51	J/mol×K	599.24	Joback Method
cpg	320.36	J/mol×K	631.30	Joback Method
cpg	329.72	J/mol×K	663.36	Joback Method
cpg	338.60	J/mol×K	695.42	Joback Method
cpg	347.00	J/mol×K	727.48	Joback Method
cpg	354.92	J/mol×K	759.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7150621&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/125-166-9/Acetic-acid-3-methylureido-ethyl-ester.pdf
Generated by Cheméo on 2024-04-25 21:54:43.759050771 +0000 UTC m=+16371332.679628086.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.