3-Ureidopropionic acid, methyl ester

Other names: Methyl N-(aminocarbonyl)-«beta»-alaninate
Inchi: InChI=1S/C5H10N2O3/c1-10-4(8)2-3-7-5(6)9/h2-3H2,1H3,(H3,6,7,9)
InchiKey: UFAMKVNXXZQVNE-UHFFFAOYSA-N
Formula: C5H10N2O3
SMILES: COC(=O)CCNC(N)=O
Mol. weight [g/mol]: 146.14

Physical Properties

Property code	Value	Unit	Source
gf	-215.78	kJ/mol	Joback Method
hf	-416.65	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.782		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
rinpol	1451.70		NIST Webbook
rinpol	1451.70		NIST Webbook
tb	566.66	K	Joback Method
tc	769.76	K	Joback Method
tf	404.12	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.73	J/mol×K	566.66	Joback Method
cpg	272.90	J/mol×K	600.51	Joback Method
cpg	281.61	J/mol×K	634.36	Joback Method
cpg	289.87	J/mol×K	668.21	Joback Method
cpg	297.67	J/mol×K	702.06	Joback Method
cpg	305.02	J/mol×K	735.91	Joback Method
cpg	311.92	J/mol×K	769.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332977&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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