Isoglutamine

Inchi: InChI=1S/C5H10N2O3/c6-3(5(7)10)1-2-4(8)9/h3H,1-2,6H2,(H2,7,10)(H,8,9)
InchiKey: AEFLONBTGZFSGQ-UHFFFAOYSA-N
Formula: C5H10N2O3
SMILES: NC(=O)C(N)CCC(=O)O
Mol. weight [g/mol]: 146.14
CAS: 328-48-3

Physical Properties

Property code	Value	Unit	Source
gf	-272.98	kJ/mol	Joback Method
hf	-461.62	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	0.23		Crippen Method
logp	-1.336		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	658.34	K	Joback Method
tc	861.60	K	Joback Method
tf	458.31	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.78	J/mol×K	658.34	Joback Method
cpg	297.34	J/mol×K	692.22	Joback Method
cpg	304.44	J/mol×K	726.09	Joback Method
cpg	311.09	J/mol×K	759.97	Joback Method
cpg	317.30	J/mol×K	793.85	Joback Method
cpg	323.09	J/mol×K	827.72	Joback Method
cpg	328.46	J/mol×K	861.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C328483&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

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