Isoasparagine

Inchi: InChI=1S/C4H8N2O3/c5-2(4(6)9)1-3(7)8/h2H,1,5H2,(H2,6,9)(H,7,8)
InchiKey: PMLJIHNCYNOQEQ-UHFFFAOYSA-N
Formula: C4H8N2O3
SMILES: NC(=O)C(N)CC(=O)O
Mol. weight [g/mol]: 132.12

Physical Properties

Property code	Value	Unit	Source
gf	-281.40	kJ/mol	Joback Method
hf	-440.98	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	0.65		Crippen Method
logp	-1.726		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
ripol	1973.00		NIST Webbook
ripol	1973.00		NIST Webbook
tb	635.46	K	Joback Method
tc	841.61	K	Joback Method
tf	447.04	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.85	J/mol×K	635.46	Joback Method
cpg	250.50	J/mol×K	669.82	Joback Method
cpg	256.73	J/mol×K	704.18	Joback Method
cpg	262.56	J/mol×K	738.53	Joback Method
cpg	268.00	J/mol×K	772.89	Joback Method
cpg	273.05	J/mol×K	807.25	Joback Method
cpg	277.73	J/mol×K	841.61	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=U130175&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume