

pro-val

Inchi: InChI=1S/C10H18N2O3/c1-6(2)8(10(14)15)12-9(13)7-4-3-5-11-7/h6-8,11H,3-5H2,1-2H3
InchiKey: AWJGUZSYVIVZGP-UHFFFAOYSA-N
Formula: C10H18N2O3
SMILES: CC(C)C(NC(=O)C1CCCN1)C(=O)O
Mol. weight [g/mol]: 214.26
CAS: 52899-09-9

Physical Properties

Property code	Value	Unit	Source
basg	909.00	kJ/mol	NIST Webbook
gf	-152.57	kJ/mol	Joback Method
hf	-485.92	kJ/mol	Joback Method
hfus	30.52	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	-0.036		Crippen Method
mcvol	169.870	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	741.24	K	Joback Method
tc	947.94	K	Joback Method
tf	501.73	K	Joback Method
vc	0.627	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.50	J/molxK	741.24	Joback Method
cpg	520.40	J/molxK	775.69	Joback Method
cpg	532.43	J/molxK	810.14	Joback Method
cpg	543.62	J/molxK	844.59	Joback Method
cpg	554.00	J/molxK	879.04	Joback Method
cpg	563.60	J/molxK	913.49	Joback Method
cpg	572.44	J/molxK	947.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52899099&Units=SI

Legend

basg:	Gas basicity
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

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