Propyl 1,2,5,6-tetrahydropyridine-3-carboxylate

Inchi: InChI=1S/C9H15NO2/c1-2-6-12-9(11)8-4-3-5-10-7-8/h4,10H,2-3,5-7H2,1H3
InchiKey: JPTZIWWBFZPVFX-UHFFFAOYSA-N
Formula: C9H15NO2
SMILES: CCCOC(=O)C1=CCCNC1
Mol. weight [g/mol]: 169.22
CAS: 251547-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-68.82	kJ/mol	Joback Method
hf	-315.11	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.859		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1588.60		NIST Webbook
rinpol	1588.60		NIST Webbook
tb	558.52	K	Joback Method
tc	775.16	K	Joback Method
tf	393.28	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.98	J/mol×K	558.52	Joback Method
cpg	349.16	J/mol×K	594.63	Joback Method
cpg	363.56	J/mol×K	630.73	Joback Method
cpg	377.17	J/mol×K	666.84	Joback Method
cpg	389.99	J/mol×K	702.95	Joback Method
cpg	402.04	J/mol×K	739.06	Joback Method
cpg	413.32	J/mol×K	775.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C251547781&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume