Pro, isopropyl ester

Inchi: InChI=1S/C8H15NO2/c1-6(2)11-8(10)7-4-3-5-9-7/h6-7,9H,3-5H2,1-2H3
InchiKey: NAHHGJMBRWRITI-UHFFFAOYSA-N
Formula: C8H15NO2
SMILES: CC(C)OC(=O)C1CCCN1
Mol. weight [g/mol]: 157.21

Physical Properties

Property code	Value	Unit	Source
gf	-95.62	kJ/mol	Joback Method
hf	-360.24	kJ/mol	Joback Method
hfus	19.27	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.690		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	522.12	K	Joback Method
tc	736.12	K	Joback Method
tf	353.01	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.14	J/mol×K	522.12	Joback Method
cpg	322.83	J/mol×K	557.79	Joback Method
cpg	337.74	J/mol×K	593.45	Joback Method
cpg	351.88	J/mol×K	629.12	Joback Method
cpg	365.24	J/mol×K	664.79	Joback Method

cpg	377.85	J/mol×K	700.45	Joback Method
cpg	389.70	J/mol×K	736.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R535869&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