Pro, propyl ester

Inchi: InChI=1S/C8H15NO2/c1-2-6-11-8(10)7-4-3-5-9-7/h7,9H,2-6H2,1H3
InchiKey: ZEERPIASPMMKRH-UHFFFAOYSA-N
Formula: C8H15NO2
SMILES: CCCOC(=O)C1CCCN1
Mol. weight [g/mol]: 157.21

Physical Properties

Property code	Value	Unit	Source
gf	-93.18	kJ/mol	Joback Method
hf	-354.96	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.692		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	1381.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	522.56	K	Joback Method
tc	731.85	K	Joback Method
tf	368.01	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.87	J/mol×K	522.56	Joback Method
cpg	322.15	J/mol×K	557.44	Joback Method
cpg	336.68	J/mol×K	592.32	Joback Method
cpg	350.49	J/mol×K	627.21	Joback Method

cpg	363.57	J/mol×K	662.09	Joback Method
cpg	375.93	J/mol×K	696.97	Joback Method
cpg	387.58	J/mol×K	731.85	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=R535918&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume