Val, propyl ester

Inchi: InChI=1S/C8H17NO2/c1-4-5-11-8(10)7(9)6(2)3/h6-7H,4-5,9H2,1-3H3
InchiKey: LVTMTRYOHIIDOO-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CCCOC(=O)C(N)C(C)C
Mol. weight [g/mol]: 159.23

Physical Properties

Property code	Value	Unit	Source
gf	-155.87	kJ/mol	Joback Method
hf	-430.02	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.923		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1154.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1167.00		NIST Webbook
tb	530.38	K	Joback Method
tc	724.15	K	Joback Method
tf	305.34	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.70	J/mol×K	530.38	Joback Method
cpg	351.98	J/mol×K	562.68	Joback Method
cpg	364.67	J/mol×K	594.97	Joback Method
cpg	376.78	J/mol×K	627.27	Joback Method
cpg	388.32	J/mol×K	659.56	Joback Method

cpg	399.29	J/mol×K	691.86	Joback Method
cpg	409.70	J/mol×K	724.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R535943&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

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