Val, isopropyl ester

Inchi: InChI=1S/C8H17NO2/c1-5(2)7(9)8(10)11-6(3)4/h5-7H,9H2,1-4H3
InchiKey: GJJLNXZGOBJOFF-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CC(C)OC(=O)C(N)C(C)C
Mol. weight [g/mol]: 159.23

Physical Properties

Property code	Value	Unit	Source
gf	-158.31	kJ/mol	Joback Method
hf	-435.30	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	52.03	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	0.921		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1112.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1126.00		NIST Webbook
tb	529.94	K	Joback Method
tc	727.82	K	Joback Method
tf	290.34	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.00	J/mol×K	529.94	Joback Method
cpg	352.62	J/mol×K	562.92	Joback Method
cpg	365.63	J/mol×K	595.90	Joback Method
cpg	378.02	J/mol×K	628.88	Joback Method
cpg	389.80	J/mol×K	661.86	Joback Method

cpg	400.99	J/mol×K	694.84	Joback Method
cpg	411.58	J/mol×K	727.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R535923&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

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