l-Norvaline, N-methoxycarbonyl-, methyl ester

Inchi: InChI=1S/C8H15NO4/c1-4-5-6(7(10)12-2)9-8(11)13-3/h6H,4-5H2,1-3H3,(H,9,11)
InchiKey: SQJRXALFHVLTQF-UHFFFAOYSA-N
Formula: C8H15NO4
SMILES: CCCC(NC(=O)OC)C(=O)OC
Mol. weight [g/mol]: 189.21

Physical Properties

Property code	Value	Unit	Source
gf	-364.41	kJ/mol	Joback Method
hf	-649.86	kJ/mol	Joback Method
hfus	23.63	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.684		Crippen Method
mcvol	148.440	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1295.00		NIST Webbook
tb	584.75	K	Joback Method
tc	773.64	K	Joback Method
tf	361.90	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.04	J/mol×K	584.75	Joback Method
cpg	382.08	J/mol×K	616.23	Joback Method
cpg	393.59	J/mol×K	647.71	Joback Method
cpg	404.56	J/mol×K	679.19	Joback Method
cpg	415.00	J/mol×K	710.67	Joback Method
cpg	424.89	J/mol×K	742.15	Joback Method
cpg	434.22	J/mol×K	773.64	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=U320768&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