Crotonylglycine, methyl ester

Inchi: InChI=1S/C7H11NO3/c1-3-4-6(9)8-5-7(10)11-2/h3-4H,5H2,1-2H3,(H,8,9)/b4-3+
InchiKey: OMXMUPFBFXABMB-ONEGZZNKSA-N
Formula: C7H11NO3
SMILES: CC=CC(=O)NCC(=O)OC
Mol. weight [g/mol]: 157.17

Physical Properties

Property code	Value	Unit	Source
gf	-185.17	kJ/mol	Joback Method
hf	-374.50	kJ/mol	Joback Method
hfus	23.57	kJ/mol	Joback Method
hvap	53.47	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	-0.148		Crippen Method
mcvol	124.180	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1524.00		NIST Webbook
tb	544.05	K	Joback Method
tc	740.95	K	Joback Method
tf	338.32	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.99	J/mol×K	544.05	Joback Method
cpg	291.40	J/mol×K	576.87	Joback Method
cpg	301.30	J/mol×K	609.68	Joback Method
cpg	310.69	J/mol×K	642.50	Joback Method
cpg	319.57	J/mol×K	675.31	Joback Method
cpg	327.98	J/mol×K	708.13	Joback Method
cpg	335.91	J/mol×K	740.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R245546&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