«alpha»-Methylbutyrylglycine, methyl ester

Inchi: InChI=1S/C8H15NO3/c1-4-6(2)8(11)9-5-7(10)12-3/h6H,4-5H2,1-3H3,(H,9,11)
InchiKey: JRTJKVMHEVDIEM-UHFFFAOYSA-N
Formula: C8H15NO3
SMILES: CCC(C)C(=O)NCC(=O)OC
Mol. weight [g/mol]: 173.21

Physical Properties

Property code	Value	Unit	Source
gf	-259.41	kJ/mol	Joback Method
hf	-517.64	kJ/mol	Joback Method
hfus	22.44	kJ/mol	Joback Method
hvap	55.35	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.322		Crippen Method
mcvol	142.570	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1296.00		NIST Webbook
tb	562.33	K	Joback Method
tc	752.51	K	Joback Method
tf	339.67	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.83	J/mol×K	562.33	Joback Method
cpg	358.00	J/mol×K	594.03	Joback Method
cpg	369.61	J/mol×K	625.72	Joback Method
cpg	380.67	J/mol×K	657.42	Joback Method
cpg	391.18	J/mol×K	689.12	Joback Method
cpg	401.15	J/mol×K	720.82	Joback Method
cpg	410.57	J/mol×K	752.51	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=R245511&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