Sarcosine, N-valeryl-, ethyl ester

Inchi: InChI=1S/C10H19NO3/c1-4-6-7-9(12)11(3)8-10(13)14-5-2/h4-8H2,1-3H3
InchiKey: TWVJCKKJOPGBOW-UHFFFAOYSA-N
Formula: C10H19NO3
SMILES: CCCCC(=O)N(C)CC(=O)OCC
Mol. weight [g/mol]: 201.26

Physical Properties

Property code	Value	Unit	Source
gf	-218.74	kJ/mol	Joback Method
hf	-539.58	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.198		Crippen Method
mcvol	170.750	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	570.80	K	Joback Method
tc	749.96	K	Joback Method
tf	357.02	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.10	J/mol×K	570.80	Joback Method
cpg	440.00	J/mol×K	600.66	Joback Method
cpg	453.27	J/mol×K	630.52	Joback Method
cpg	465.92	J/mol×K	660.38	Joback Method
cpg	477.96	J/mol×K	690.24	Joback Method
cpg	489.40	J/mol×K	720.10	Joback Method
cpg	500.26	J/mol×K	749.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321559&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