Sarcosine, n-valeryl-, propyl ester

Inchi: InChI=1S/C11H21NO3/c1-4-6-7-10(13)12(3)9-11(14)15-8-5-2/h4-9H2,1-3H3
InchiKey: XYLPTBMTYSRXOJ-UHFFFAOYSA-N
Formula: C11H21NO3
SMILES: CCCCC(=O)N(C)CC(=O)OCCC
Mol. weight [g/mol]: 215.29

Physical Properties

Property code	Value	Unit	Source
hf	-679.84	kJ/mol	Cheméo Relay (1.0)
hfus	31.65	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-1.20		Cheméo Relay (1.0)
logp	1.588		Crippen Method
mcvol	184.840	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
tb	537.38	K	Cheméo Relay (1.0)
tc	708.63	K	Cheméo Relay (1.0)
tf	251.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.61	J/mol×K	593.68	Joback Method
cpg	490.16	J/mol×K	623.29	Joback Method
cpg	504.05	J/mol×K	652.90	Joback Method
cpg	517.27	J/mol×K	682.51	Joback Method
cpg	529.86	J/mol×K	712.12	Joback Method
cpg	541.81	J/mol×K	741.73	Joback Method
cpg	553.15	J/mol×K	771.34	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321560&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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