L-alanine, n-caproyl-, methyl ester

Inchi: InChI=1S/C10H19NO3/c1-4-5-6-7-9(12)11-8(2)10(13)14-3/h8H,4-7H2,1-3H3,(H,11,12)
InchiKey: ZHXNJDXOOUINCL-UHFFFAOYSA-N
Formula: C10H19NO3
SMILES: CCCCCC(=O)NC(C)C(=O)OC
Mol. weight [g/mol]: 201.27

Physical Properties

Property code	Value	Unit	Source
hf	-694.23	kJ/mol	Cheméo Relay (1.0)
hfus	27.62	kJ/mol	Joback Method
hvap	72.66	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-1.72		Cheméo Relay (1.0)
logp	1.244		Crippen Method
mcvol	170.750	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1451.00		NIST Webbook
tb	509.19	K	Cheméo Relay (1.0)
tc	709.69	K	Cheméo Relay (1.0)
tf	324.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.06	J/mol×K	608.09	Joback Method
cpg	455.73	J/mol×K	639.09	Joback Method
cpg	468.75	J/mol×K	670.09	Joback Method
cpg	481.12	J/mol×K	701.09	Joback Method
cpg	492.87	J/mol×K	732.09	Joback Method
cpg	503.99	J/mol×K	763.08	Joback Method
cpg	514.49	J/mol×K	794.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299732&Units=SI
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):	

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