L-Norvaline, N-propoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C18H35NO4/c1-4-7-8-9-10-11-12-15-22-17(20)16(13-5-2)19-18(21)23-14-6-3/h
InchiKey: KIGOGYGOAMKMEC-UHFFFAOYSA-N
Formula: C18H35NO4
SMILES: CCCCCCCCCOC(=O)C(CCC)NC(=O)OCCC
Mol. weight [g/mol]: 329.48

Physical Properties

Property code	Value	Unit	Source
hfus	49.53	kJ/mol	Joback Method
hvap	97.12	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.91		Cheméo Relay (1.0)
logp	4.585		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	597.07	K	Cheméo Relay (1.0)
tc	789.56	K	Cheméo Relay (1.0)
tf	292.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.06	J/mol×K	813.55	Joback Method
cpg	930.15	J/mol×K	844.64	Joback Method
cpg	946.21	J/mol×K	875.74	Joback Method
cpg	961.26	J/mol×K	906.83	Joback Method
cpg	975.31	J/mol×K	937.93	Joback Method
cpg	988.37	J/mol×K	969.02	Joback Method
cpg	1000.48	J/mol×K	1000.12	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320735&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

Legend

cpg:	Ideal gas heat capacity
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