l-Norvaline, n-butoxycarbonyl-, octyl ester

Inchi: InChI=1S/C18H35NO4/c1-4-7-9-10-11-12-15-22-17(20)16(13-6-3)19-18(21)23-14-8-5-2/l
InchiKey: DKAFIYFGRXDWDP-UHFFFAOYSA-N
Formula: C18H35NO4
SMILES: CCCCCCCCOC(=O)C(CCC)NC(=O)OCCCC
Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
gf	-280.21	kJ/mol	Joback Method
hf	-856.26	kJ/mol	Joback Method
hfus	49.53	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.585		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	1996.00		NIST Webbook
tb	813.55	K	Joback Method
tc	1000.12	K	Joback Method
tf	474.60	K	Joback Method
vc	1.121	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320776&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

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