Glycine, N-methyl-n-butoxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C26H51NO4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-30-25(28)24

InchiKey: CDAKSSJKNOGRDZ-UHFFFAOYSA-N

Formula: C26H51NO4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)OCCCC

Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
gf	-189.02	kJ/mol	Joback Method
hf	-1002.04	kJ/mol	Joback Method
hfus	71.69	kJ/mol	Joback Method
hvap	93.83	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.660		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	761.42	kPa	Joback Method
rinpol	2833.00		NIST Webbook
rinpol	2833.00		NIST Webbook
tb	959.30	K	Joback Method
tc	1184.49	K	Joback Method
tf	559.57	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.27	J/mol×K	959.30	Joback Method
cpg	1412.01	J/mol×K	996.83	Joback Method
cpg	1431.99	J/mol×K	1034.36	Joback Method
cpg	1450.29	J/mol×K	1071.90	Joback Method
cpg	1466.96	J/mol×K	1109.43	Joback Method
cpg	1482.08	J/mol×K	1146.96	Joback Method
cpg	1495.71	J/mol×K	1184.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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