D-Alanine, N-butoxycarbonyl-, octyl ester

Inchi: InChI=1S/C16H31NO4/c1-4-6-8-9-10-11-13-20-15(18)14(3)17-16(19)21-12-7-5-2/h14H,4
InchiKey: SNAUXJXTALTNGV-UHFFFAOYSA-N
Formula: C16H31NO4
SMILES: CCCCCCCCOC(=O)C(C)NC(=O)OCCCC
Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-297.05	kJ/mol	Joback Method
hf	-814.98	kJ/mol	Joback Method
hfus	44.35	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.805		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	767.79	K	Joback Method
tc	950.65	K	Joback Method
tf	452.06	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.32	J/mol×K	767.79	Joback Method
cpg	811.65	J/mol×K	798.27	Joback Method
cpg	827.08	J/mol×K	828.74	Joback Method
cpg	841.60	J/mol×K	859.22	Joback Method
cpg	855.22	J/mol×K	889.70	Joback Method
cpg	867.97	J/mol×K	920.17	Joback Method
cpg	879.84	J/mol×K	950.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347722&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