D-Alanine, N-neopentyloxycarbonyl-, heptyl ester

Inchi: InChI=1S/C16H31NO4/c1-6-7-8-9-10-11-20-14(18)13(2)17-15(19)21-12-16(3,4)5/h13H,6

InchiKey: LNOCTUQYKQZVRP-UHFFFAOYSA-N

Formula: C16H31NO4

SMILES: CCCCCCCOC(=O)C(C)NC(=O)OCC(C)(C)C

Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-294.21	kJ/mol	Joback Method
hf	-823.73	kJ/mol	Joback Method
hfus	36.93	kJ/mol	Joback Method
hvap	74.27	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.661		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	1941.00		NIST Webbook
tb	764.56	K	Joback Method
tc	952.13	K	Joback Method
tf	454.48	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.98	J/mol×K	764.56	Joback Method
cpg	813.48	J/mol×K	795.82	Joback Method
cpg	829.02	J/mol×K	827.08	Joback Method
cpg	843.63	J/mol×K	858.34	Joback Method
cpg	857.32	J/mol×K	889.61	Joback Method
cpg	870.12	J/mol×K	920.87	Joback Method
cpg	882.06	J/mol×K	952.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347765&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

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