D-Alanine, N-neopentyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C17H33NO4/c1-6-7-8-9-10-11-12-21-15(19)14(2)18-16(20)22-13-17(3,4)5/h14

InchiKey: HYHURVUCXNHNBI-UHFFFAOYSA-N

Formula: C17H33NO4

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

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-285.79	kJ/mol	Joback Method
hf	-844.37	kJ/mol	Joback Method
hfus	39.52	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.051		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	2038.00		NIST Webbook
rinpol	2038.00		NIST Webbook
tb	787.44	K	Joback Method
tc	975.66	K	Joback Method
tf	465.75	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.13	J/mol×K	787.44	Joback Method
cpg	871.94	J/mol×K	818.81	Joback Method
cpg	887.75	J/mol×K	850.18	Joback Method
cpg	902.59	J/mol×K	881.55	Joback Method
cpg	916.48	J/mol×K	912.92	Joback Method
cpg	929.45	J/mol×K	944.29	Joback Method
cpg	941.53	J/mol×K	975.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347766&Units=SI

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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