D-Alanine, N-neopentyloxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C13H25NO4/c1-9(2)7-17-11(15)10(3)14-12(16)18-8-13(4,5)6/h9-10H,7-8H2,1-

InchiKey: KPIPBWFYJRHDQT-UHFFFAOYSA-N

Formula: C13H25NO4

SMILES: CC(C)COC(=O)C(C)NC(=O)OCC(C)(C)C

Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-321.91	kJ/mol	Joback Method
hf	-767.09	kJ/mol	Joback Method
hfus	25.64	kJ/mol	Joback Method
hvap	67.21	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.346		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	695.48	K	Joback Method
tc	887.25	K	Joback Method
tf	405.67	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.14	J/mol×K	695.48	Joback Method
cpg	644.86	J/mol×K	727.44	Joback Method
cpg	659.69	J/mol×K	759.40	Joback Method
cpg	673.64	J/mol×K	791.36	Joback Method
cpg	686.73	J/mol×K	823.32	Joback Method
cpg	698.99	J/mol×K	855.28	Joback Method
cpg	710.42	J/mol×K	887.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347762&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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