

D-Isoleucine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi:	InChI=1S/C14H27NO4/c1-7-10(5)12(15-14(17)18-8-2)13(16)19-11(6)9(3)4/h9-12H,7-8H
InchiKey:	CBNGHOBZNGEELV-MOENNCHZSA-N
Formula:	C14H27NO4
SMILES:	CCOC(=O)NC(C(=O)OC(C)C(C)C)C(C)CC
Mol. weight [g/mol]:	273.37

Physical Properties

Property code	Value	Unit	Source
gf	-321.21	kJ/mol	Joback Method
hf	-789.54	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.735		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	1647.40		NIST Webbook
rinpol	1671.10		NIST Webbook
rinpol	1647.40		NIST Webbook
tb	720.71	K	Joback Method
tc	909.23	K	Joback Method
tf	384.52	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.96	J/molxK	720.71	Joback Method
cpg	699.14	J/molxK	752.13	Joback Method
cpg	714.43	J/molxK	783.55	Joback Method
cpg	728.81	J/molxK	814.97	Joback Method
cpg	742.31	J/molxK	846.39	Joback Method
cpg	754.92	J/molxK	877.81	Joback Method
cpg	766.65	J/molxK	909.23	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=R501856&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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