

L-Isoleucine, ethyl ester

Other names:	Isoleucine, ethyl ester, L-ethyl L-isoleucinate Isoleucine ethyl ester
Inchi:	InChI=1S/C8H17NO2/c1-4-6(3)7(9)8(10)11-5-2/h6-7H,4-5,9H2,1-3H3
InchiKey:	ICPWNTVICOHCML-UHFFFAOYSA-N
Formula:	C8H17NO2
SMILES:	CCOC(=O)C(N)C(C)CC
Mol. weight [g/mol]:	159.23
CAS:	921-74-4

Physical Properties

Property code	Value	Unit	Source
af	0.5086		Cheméo Relay (1.0)
hf	-523.44	kJ/mol	Cheméo Relay (1.0)
hfus	17.41	kJ/mol	Joback Method
hvap	57.98	kJ/mol	Cheméo Relay (1.0)
ie	8.45	eV	Cheméo Relay (1.0)
log10ws	-1.67		Cheméo Relay (1.0)
logp	0.923		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
tb	444.28	K	Cheméo Relay (1.0)
tc	639.97	K	Cheméo Relay (1.0)
tf	293.66	K	Cheméo Relay (1.0)
vc	0.493	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.70	J/mol×K	530.38	Joback Method
cpg	351.98	J/mol×K	562.68	Joback Method
cpg	364.67	J/mol×K	594.97	Joback Method

cpg	376.78	J/mol×K	627.27	Joback Method
cpg	388.32	J/mol×K	659.56	Joback Method
cpg	399.29	J/mol×K	691.86	Joback Method
cpg	409.70	J/mol×K	724.15	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55056627&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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