

DL-3-aminoisobutyric acid, methyl ester

Other names:	Methyl 3-amino-2-methylpropanoate
Inchi:	InChI=1S/C5H11NO2/c1-4(3-6)5(7)8-2/h4H,3,6H2,1-2H3
InchiKey:	BXGDNKQFNQZCLG-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	COC(=O)C(C)CN
Mol. weight [g/mol]:	117.15

Physical Properties

Property code	Value	Unit	Source
af	0.4608		Cheméo Relay (1.0)
hf	-436.53	kJ/mol	Cheméo Relay (1.0)
hfus	13.17	kJ/mol	Joback Method
hvap	49.83	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
logp	-0.246		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	902.20		NIST Webbook
tb	414.50	K	Cheméo Relay (1.0)
tc	598.35	K	Cheméo Relay (1.0)
tf	286.75	K	Cheméo Relay (1.0)
vc	0.344	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.74	J/mol×K	462.18	Joback Method
cpg	220.39	J/mol×K	494.99	Joback Method
cpg	229.66	J/mol×K	527.81	Joback Method
cpg	238.56	J/mol×K	560.62	Joback Method
cpg	247.09	J/mol×K	593.43	Joback Method
cpg	255.24	J/mol×K	626.24	Joback Method
cpg	263.02	J/mol×K	659.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U332881&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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