

N-cyanomethyl-beta-iso-butylamino propionic acid, methyl ester

Inchi:	InChI=1S/C10H18N2O2/c1-9(2)8-12(7-5-11)6-4-10(13)14-3/h9H,4,6-8H2,1-3H3
InchiKey:	IKDGSHMETZGTKU-UHFFFAOYSA-N
Formula:	C10H18N2O2
SMILES:	COC(=O)CCN(CC#N)CC(C)C
Mol. weight [g/mol]:	198.26
CAS:	116295-98-8

Physical Properties

Property code	Value	Unit	Source
gf	40.92	kJ/mol	Joback Method
hf	-267.40	kJ/mol	Joback Method
hfus	25.45	kJ/mol	Joback Method
hvap	59.14	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.031		Crippen Method
mcvol	170.560	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
tb	618.57	K	Joback Method
tc	808.25	K	Joback Method
tf	357.08	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.64	J/molxK	618.57	Joback Method
cpg	453.74	J/molxK	650.18	Joback Method
cpg	466.18	J/molxK	681.80	Joback Method
cpg	477.97	J/molxK	713.41	Joback Method
cpg	489.13	J/molxK	745.02	Joback Method
cpg	499.67	J/molxK	776.63	Joback Method
cpg	509.61	J/molxK	808.25	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=C116295988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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