

«gamma»-Aminobutyric acid, N-isobutoxycarbonyl-, hexyl ester

Other names: .gamma.-Aminobutyric acid, N-isobutoxycarbonyl-, hexyl ester

Inchi: InChI=1S/C15H29NO4/c1-4-5-6-7-11-19-14(17)9-8-10-16-15(18)20-12-13(2)3/h13H,4-12

InchiKey: PMYXWNLDNNSWBB-UHFFFAOYSA-N

Formula: C₁₅H₂₉NO₄

SMILES: CCCCCOC(=O)CCCN(C(=O)OCC(C)C)C

Mol. weight [g/mol]: 287.40

Physical Properties

Property code	Value	Unit	Source
gf	-305.47	kJ/mol	Joback Method
hf	-794.34	kJ/mol	Joback Method
hfus	41.76	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.272		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2061.00		NIST Webbook
rinpol	2061.00		NIST Webbook
tb	744.91	K	Joback Method
tc	926.88	K	Joback Method
tf	440.79	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.86	J/mol×K	744.91	Joback Method
cpg	753.81	J/mol×K	775.24	Joback Method
cpg	768.89	J/mol×K	805.57	Joback Method
cpg	783.13	J/mol×K	835.90	Joback Method
cpg	796.51	J/mol×K	866.22	Joback Method
cpg	809.06	J/mol×K	896.55	Joback Method
cpg	820.77	J/mol×K	926.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinsol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/22-877-4/gamma-Aminobutyric-acid-N-isobutoxycarbonyl-hexyl-ester.pdf>

Generated by Cheméo on 2025-12-05 22:31:59.904781199 +0000 UTC m=+4722117.434821857.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.