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

Other names: .gama.-Aminobutyric acid, N-isobutoxycarbonyl-, decyl ester
Inchi: InChI=1S/C19H37NO4/c1-4-5-6-7-8-9-10-11-15-23-18(21)13-12-14-20-19(22)24-16-17(2
InchiKey: VGKJDELCRLYRJP-UHFFFAOYSA-N
Formula: C19H37NO4
SMILES: CCCCCCCCCCOC(=O)CCCNC(=O)OCC(C)C
Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
gf	-271.79	kJ/mol	Joback Method
hf	-876.90	kJ/mol	Joback Method
hfus	52.12	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.833		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2468.00		NIST Webbook
rinpol	2468.00		NIST Webbook
tb	836.43	K	Joback Method
tc	1025.94	K	Joback Method
tf	485.87	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.19	J/mol×K	836.43	Joback Method
cpg	990.66	J/mol×K	868.01	Joback Method
cpg	1007.04	J/mol×K	899.60	Joback Method
cpg	1022.33	J/mol×K	931.18	Joback Method
cpg	1036.57	J/mol×K	962.77	Joback Method
cpg	1049.77	J/mol×K	994.35	Joback Method
cpg	1061.95	J/mol×K	1025.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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