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

Other names: .gama.-Aminobutyric acid, N-isobutoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C26H51NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-30-25(28)20-19-2

InchiKey: RGQFMKNSSWBYBX-UHFFFAOYSA-N

Formula: C26H51NO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCNC(=O)OCC(C)C

Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
gf	-212.85	kJ/mol	Joback Method
hf	-1021.38	kJ/mol	Joback Method
hfus	70.25	kJ/mol	Joback Method
hvap	97.83	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.563		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	771.18	kPa	Joback Method
tb	996.59	K	Joback Method
tc	1233.25	K	Joback Method
tf	564.76	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1411.28	J/mol×K	996.59	Joback Method
cpg	1432.12	J/mol×K	1036.03	Joback Method
cpg	1451.03	J/mol×K	1075.48	Joback Method
cpg	1468.07	J/mol×K	1114.92	Joback Method
cpg	1483.30	J/mol×K	1154.36	Joback Method
cpg	1496.80	J/mol×K	1193.81	Joback Method
cpg	1508.63	J/mol×K	1233.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321059&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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