.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]: 441.70

Physical Properties

Property code	Value	Unit	Source
hf	-1209.42	kJ/mol	Cheméo Relay (1.0)
hfus	70.25	kJ/mol	Joback Method
hvap	131.14	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.00		Cheméo Relay (1.0)
logp	7.563		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	771.18	kPa	Joback Method
tb	669.89	K	Cheméo Relay (1.0)
tc	858.02	K	Cheméo Relay (1.0)
tf	313.30	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321059&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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