Propionic acid, 2-benzamido-3,3'-thiodi-, diethyl ester

Inchi: InChI=1S/C17H23NO5S/c1-3-22-15(19)10-11-24-12-14(17(21)23-4-2)18-16(20)13-8-6-5-
InchiKey: XAJHKKNIXXMYJX-UHFFFAOYSA-N
Formula: C17H23NO5S
SMILES: CCOC(=O)CCSCC(NC(=O)c1ccccc1)C(=O)OCC
Mol. weight [g/mol]: 353.43

Physical Properties

Property code	Value	Unit	Source
gf	-272.02	kJ/mol	Joback Method
hf	-669.80	kJ/mol	Joback Method
hfus	46.71	kJ/mol	Joback Method
hvap	93.63	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.035		Crippen Method
mcvol	269.410	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
tb	940.00	K	Joback Method
tc	1164.83	K	Joback Method
tf	574.08	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.50	J/mol×K	940.00	Joback Method
cpg	839.79	J/mol×K	977.47	Joback Method
cpg	849.73	J/mol×K	1014.94	Joback Method
cpg	858.32	J/mol×K	1052.41	Joback Method
cpg	865.60	J/mol×K	1089.89	Joback Method
cpg	871.59	J/mol×K	1127.36	Joback Method
cpg	876.29	J/mol×K	1164.83	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=B6008265&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