2-Aminoadipic acid, N-trifluoroacetyl-, di-n-butyl ester

Other names: Adipic acid, 2-amino, butyl ester, TFA
Inchi: InChI=1S/C16H26F3NO5/c1-3-5-10-24-13(21)9-7-8-12(14(22)25-11-6-4-2)20-15(23)16(1
InchiKey: NPYXALIPFYRYAQ-UHFFFAOYSA-N
Formula: C16H26F3NO5
SMILES: CCCCOC(=O)CCCC(NC(=O)C(F)(F)F)C(=O)OCCCC
Mol. weight [g/mol]: 369.38

Physical Properties

Property code	Value	Unit	Source
gf	-1007.56	kJ/mol	Joback Method
hf	-1524.64	kJ/mol	Joback Method
hfus	47.77	kJ/mol	Joback Method
hvap	78.57	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.890		Crippen Method
mcvol	268.040	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
rinpol	1868.00		NIST Webbook
tb	816.24	K	Joback Method
tc	1002.46	K	Joback Method
tf	506.18	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.26	J/mol×K	816.24	Joback Method
cpg	853.24	J/mol×K	847.28	Joback Method
cpg	866.29	J/mol×K	878.31	Joback Method
cpg	878.43	J/mol×K	909.35	Joback Method
cpg	889.69	J/mol×K	940.39	Joback Method
cpg	900.10	J/mol×K	971.42	Joback Method
cpg	909.68	J/mol×K	1002.46	Joback Method

Sources

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=U328293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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