2,4-diaminobutanoic acid, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C11H14F6N2O4/c1-5(2)23-7(20)6(19-9(22)11(15,16)17)3-4-18-8(21)10(12,13)

InchiKey: QPYOLYVWVHLBGA-UHFFFAOYSA-N

Formula: C11H14F6N2O4

SMILES: CC(C)OC(=O)C(CCNC(=O)C(F)(F)F)NC(=O)C(F)(F)F

Mol. weight [g/mol]: 352.23

Physical Properties

Property code	Value	Unit	Source
gf	-1439.30	kJ/mol	Joback Method
hf	-1838.11	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	67.33	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	1.054		Crippen Method
mcvol	207.010	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	723.73	K	Joback Method
tc	900.35	K	Joback Method
tf	469.45	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.93	J/mol×K	723.73	Joback Method
cpg	627.68	J/mol×K	753.17	Joback Method
cpg	637.71	J/mol×K	782.60	Joback Method
cpg	647.04	J/mol×K	812.04	Joback Method
cpg	655.71	J/mol×K	841.48	Joback Method
cpg	663.76	J/mol×K	870.91	Joback Method
cpg	671.22	J/mol×K	900.35	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=R267808&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