«beta»-Alanine, n-heptafluorobutyryl-, butyl ester

Inchi: InChI=1S/C11H14F7NO3/c1-2-3-6-22-7(20)4-5-19-8(21)9(12,13)10(14,15)11(16,17)18/h

InchiKey: CACSVWBMQVQIBE-UHFFFAOYSA-N

Formula: C11H14F7NO3

SMILES: CCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 341.22

Physical Properties

Property code	Value	Unit	Source
gf	-1586.86	kJ/mol	Joback Method
hf	-1973.30	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	52.81	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.669		Crippen Method
mcvol	197.230	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1334.00		NIST Webbook
rinpol	1334.00		NIST Webbook
tb	616.61	K	Joback Method
tc	777.42	K	Joback Method
tf	399.87	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.02	J/mol×K	616.61	Joback Method
cpg	569.96	J/mol×K	643.41	Joback Method
cpg	581.17	J/mol×K	670.21	Joback Method
cpg	591.70	J/mol×K	697.01	Joback Method
cpg	601.58	J/mol×K	723.81	Joback Method
cpg	610.84	J/mol×K	750.62	Joback Method
cpg	619.53	J/mol×K	777.42	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=U320979&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