.beta.-Alanine, N-pentafluoropropionyl-, isobutyl ester

Inchi: InChI=1S/C10H14F5NO3/c1-6(2)5-19-7(17)3-4-16-8(18)9(11,12)10(13,14)15/h6H,3-5H2

InchiKey: QAUNVMSVKLBRER-UHFFFAOYSA-N

Formula: C10H14F5NO3

SMILES: CC(C)COC(=O)CCNC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 291.22

Physical Properties

Property code	Value	Unit	Source
hf	-1743.76	kJ/mol	Cheméo Relay (1.0)
hfus	28.19	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Cheméo Relay (1.0)
ie	10.29	eV	Cheméo Relay (1.0)
logp	1.889		Crippen Method
mcvol	179.600	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1266.00		NIST Webbook
rinpol	1266.00		NIST Webbook
tb	484.41	K	Cheméo Relay (1.0)
tc	623.94	K	Cheméo Relay (1.0)
tf	295.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.24	J/mol×K	597.98	Joback Method
cpg	501.32	J/mol×K	625.97	Joback Method
cpg	512.71	J/mol×K	653.97	Joback Method
cpg	523.43	J/mol×K	681.96	Joback Method
cpg	533.51	J/mol×K	709.96	Joback Method
cpg	542.99	J/mol×K	737.95	Joback Method
cpg	551.89	J/mol×K	765.95	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320949&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

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
ie:	Ionization energy
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