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

Inchi: InChI=1S/C14H20F7NO3/c1-2-3-4-5-6-9-25-10(23)7-8-22-11(24)12(15,16)13(17,18)14(1

InchiKey: ZBOYVKZCKRZEKQ-UHFFFAOYSA-N

Formula: C14H20F7NO3

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

Mol. weight [g/mol]: 383.30

Physical Properties

Property code	Value	Unit	Source
gf	-1561.60	kJ/mol	Joback Method
hf	-2035.22	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	59.49	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.839		Crippen Method
mcvol	239.500	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
tb	685.25	K	Joback Method
tc	848.74	K	Joback Method
tf	433.68	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.58	J/mol×K	685.25	Joback Method
cpg	727.88	J/mol×K	712.50	Joback Method
cpg	740.40	J/mol×K	739.75	Joback Method
cpg	752.18	J/mol×K	766.99	Joback Method
cpg	763.27	J/mol×K	794.24	Joback Method
cpg	773.71	J/mol×K	821.49	Joback Method
cpg	783.53	J/mol×K	848.74	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=U320982&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